High Performance Computing (HPC) at UL

Present and Future Challenges

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UL HPC Management Team,

Parallel Computing and Optimization Group (PCOG),

University of Luxembourg (UL), Luxembourg

Summary

1 Preliminaries

2 The UL HPC platform
Overview
Platform Management Tools
Monitoring
Statistics & Milestones

3 Incoming Milestones and Challenges

Computing / Storage Performances

- **HPC**: **H**igh **P**erformance **C**omputing

Main HPC Performance Metrics

- Computing Capacity/speed: often measured in **flops** (or **flop/s**)
  - ↪ **Fl**oating **p**oint **o**perations per **s**econds (often in DP)
  - ↪ **GFlops** $= 10^9$ Flops **TFlops** $= 10^{12}$ Flops **PFlops** $= 10^{15}$ Flops
- Storage Capacity measured in multiples of **bytes** $= 8$ **bits**
  - ↪ **GB** $= 10^9$ bytes **TB** $= 10^{12}$ bytes **PB** $= 10^{15}$ bytes
  - ↪ **GiB** $= 1024^3$ bytes **TiB** $= 1024^4$ bytes **PiB** $= 1024^5$ bytes
- Transfer rate on a medium measured in **Mb/s** or **MB/s**
- Other metrics: Sequential vs Random **R/W speed**, **IOPS**

Why High Performance Computing ?

"The country that out-computes will be the one that out-competes". *Council on Competitiveness*

- Accelerate research by accelerating **computations**

14.4 **G**Flops (Dual-core i7 1.8GHz)

49.918**T**Flops (400computing nodes, 4284cores)

- Increase **storage** capacity

2TB (1 disk)

4268.4TB raw(642disks)

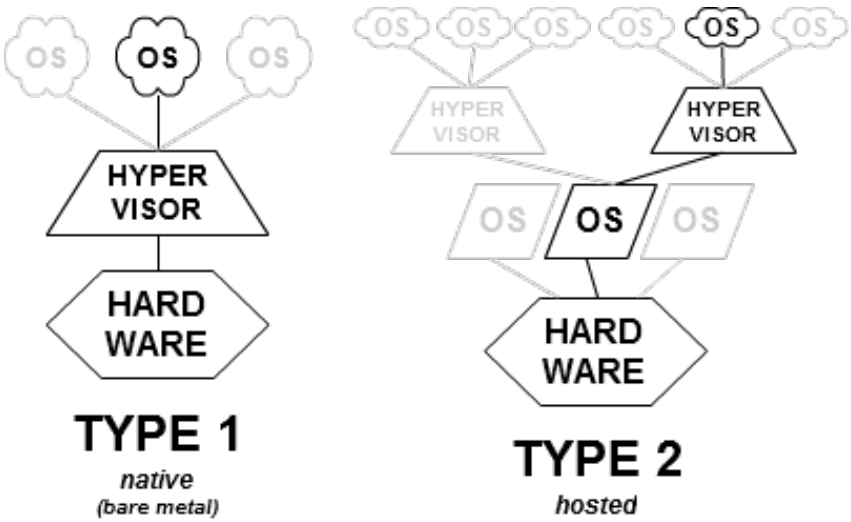
- Communicate **faster** 1 GbE (1 Gb/s) vs Infiniband QDR (40 Gb/s)

Computing for Researchers

- Regular PC / Local Laptop / Workstation
  - ↪ Native OS (Windows, Linux, Mac etc.)

Computing for Researchers

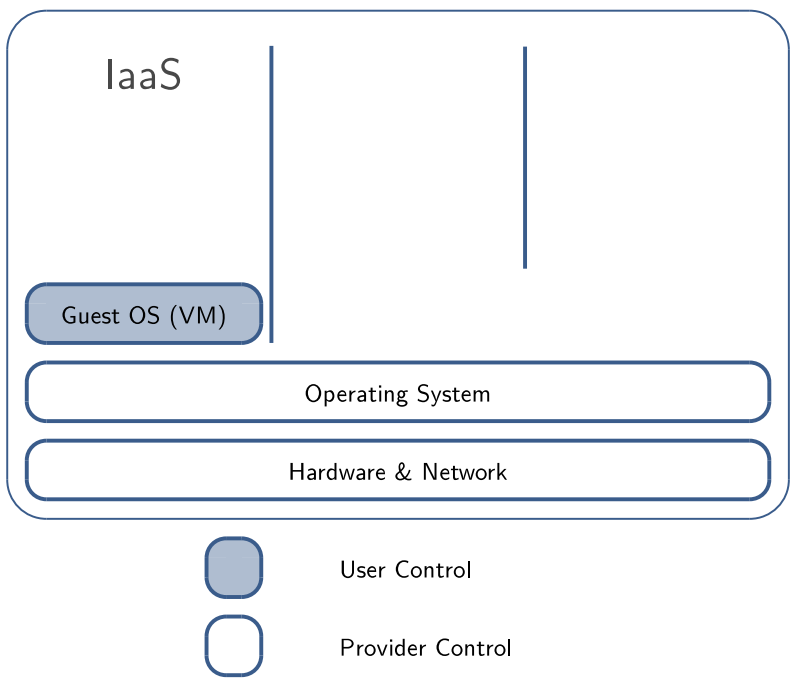
- Regular PC / Local Laptop / Workstation
  - ↪ Native OS (Windows, Linux, Mac etc.)
  - ↪ Virtualized OS through an **hypervisor**
    - ✓ Hypervisor: core virtualization engine / environment
    - ✓ **Performance loss:** $\geq 20\%$



Xen, VMWare ESXi, KVM VirtualBox

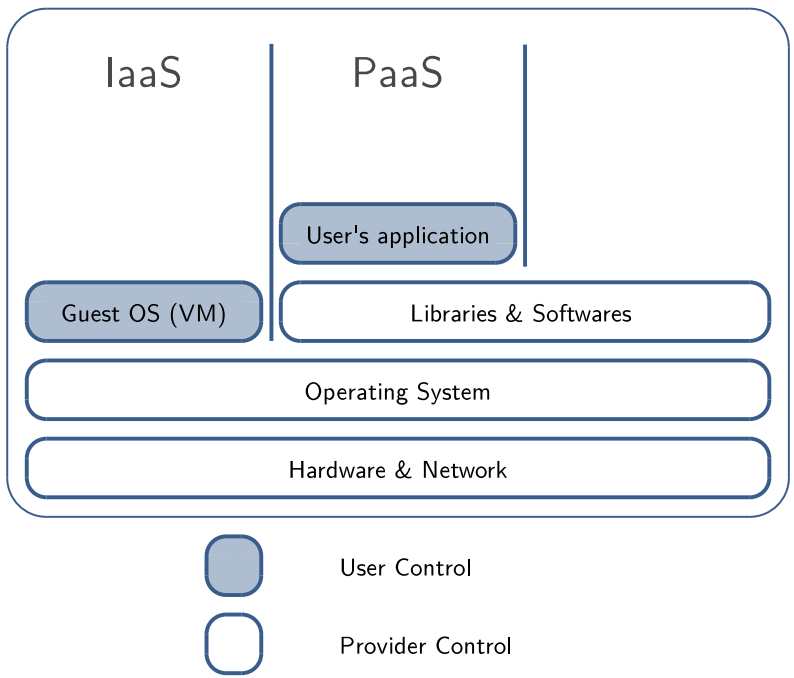
Computing for Researchers

- Cloud Computing Platform
  - ↪ **Infrastructure** as a Service (IaaS)



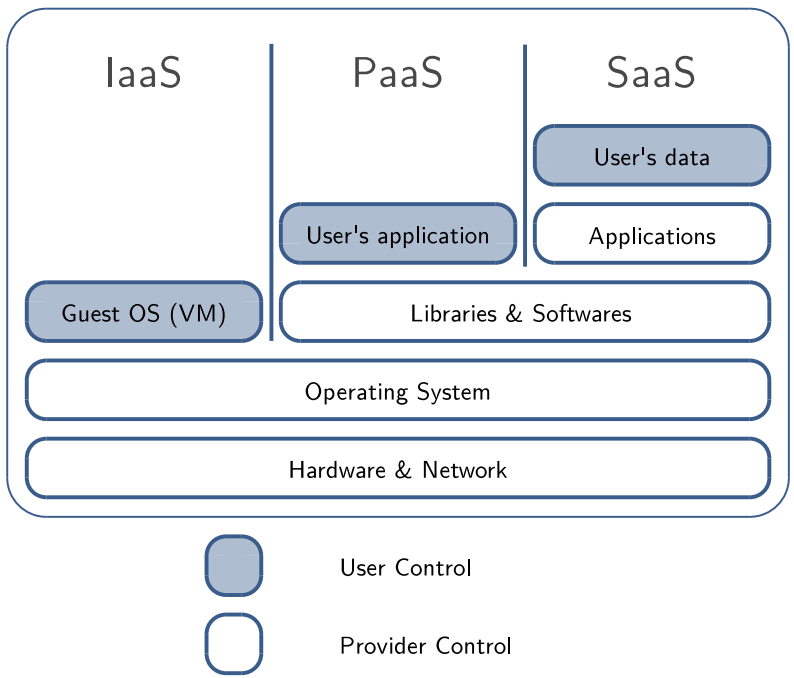
Computing for Researchers

- Cloud Computing Platform
  - ↪ **Platform** as a Service (PaaS)



Computing for Researchers

- Cloud Computing Platform
  - ↪ **Software** as a Service (SaaS)



Computing for Researchers

- High Performance Computing platforms
  - ↪ For **Speedup**, **Scalability** and **Faster Time to Solution**

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YET...

$$\textbf{PC} \neq \textbf{HPC}$$

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YET...

PC $\neq$ HPC

- HPC $\simeq$ Formula 1
  - ↪ can end badly, even after minor errors

Jobs, Tasks & Local Execution

```
$> ./myprog
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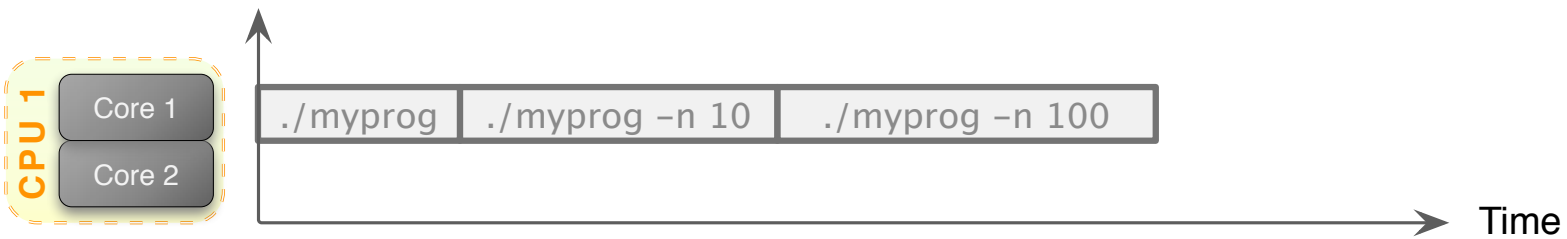

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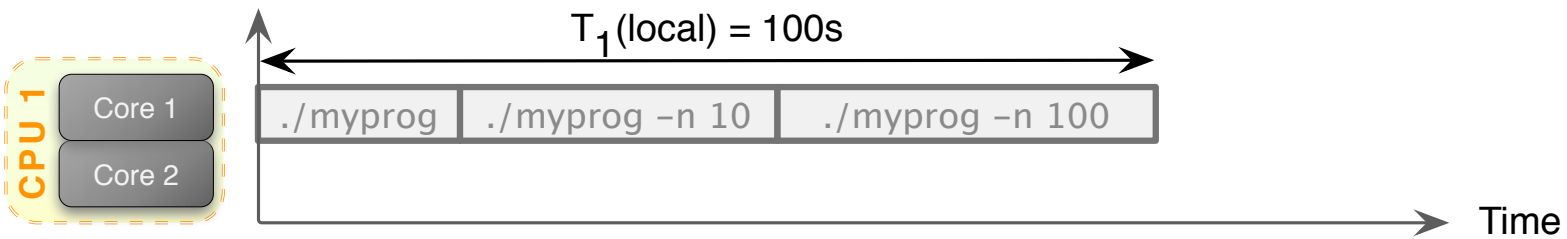

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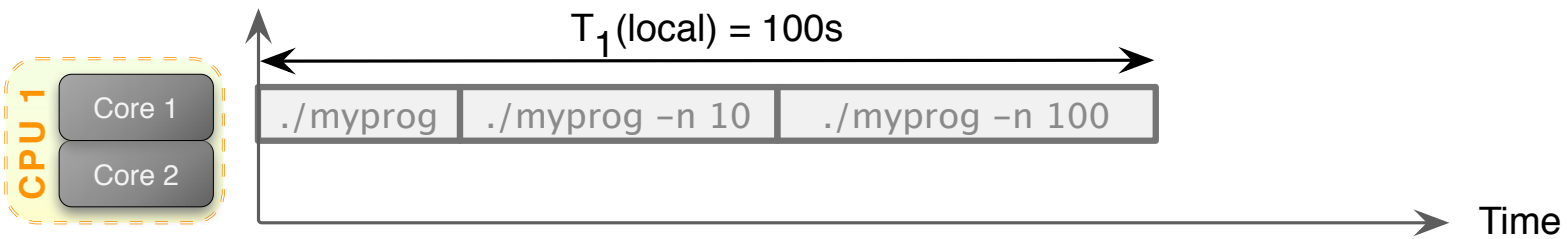
Job(s) 3

Task(s) 3



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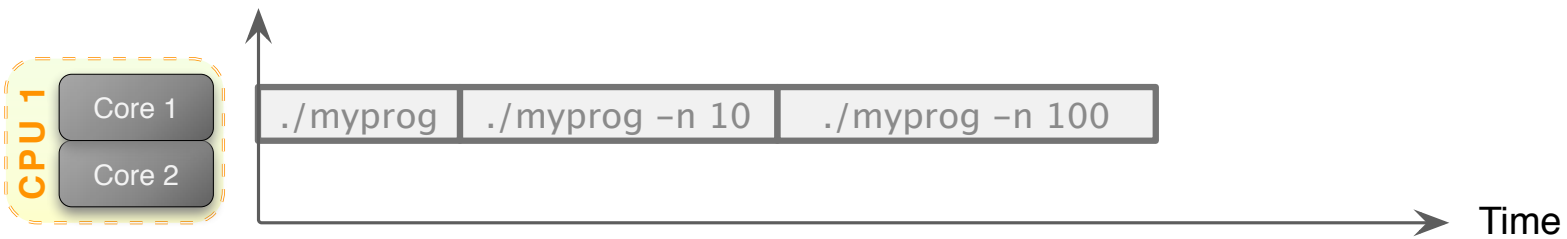

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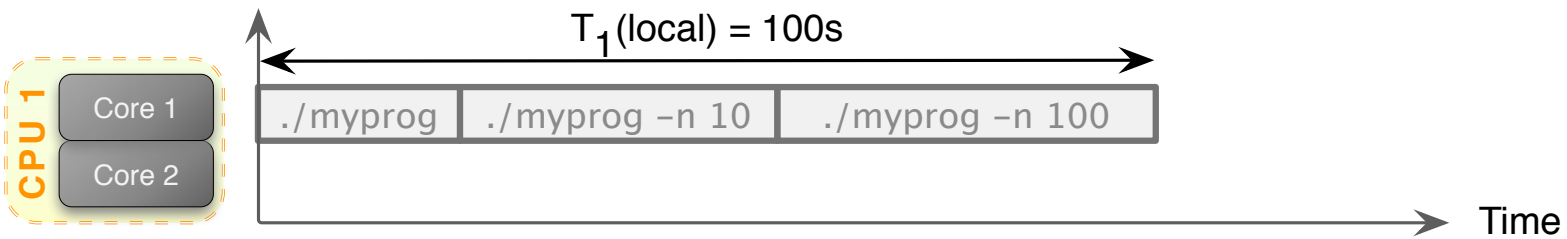

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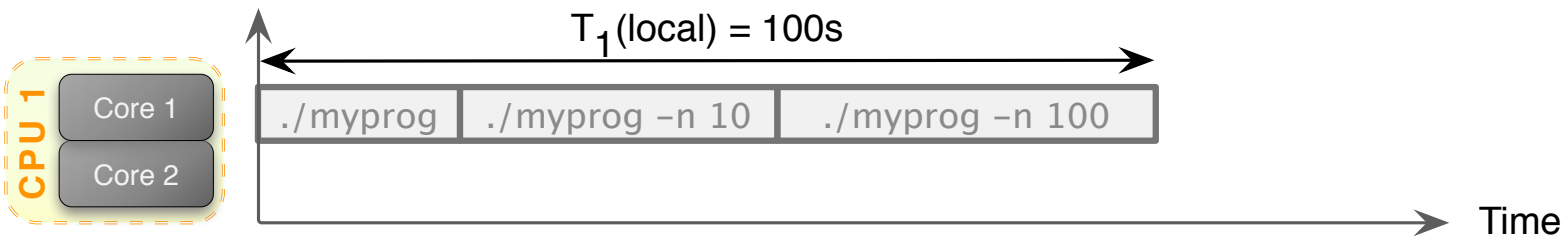

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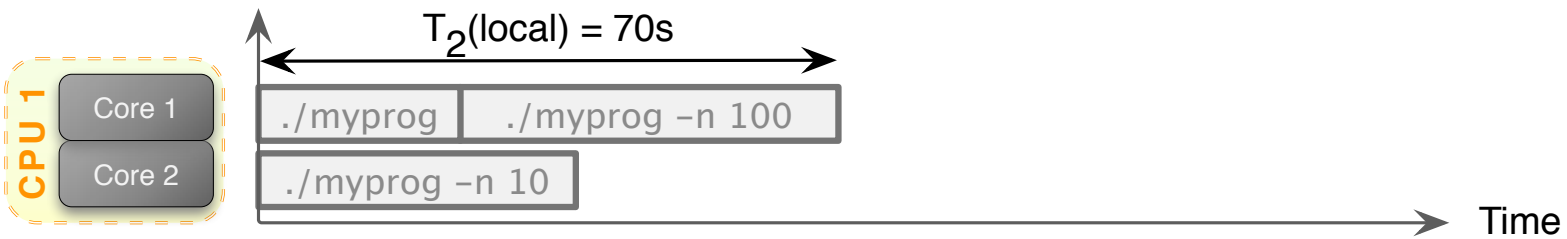

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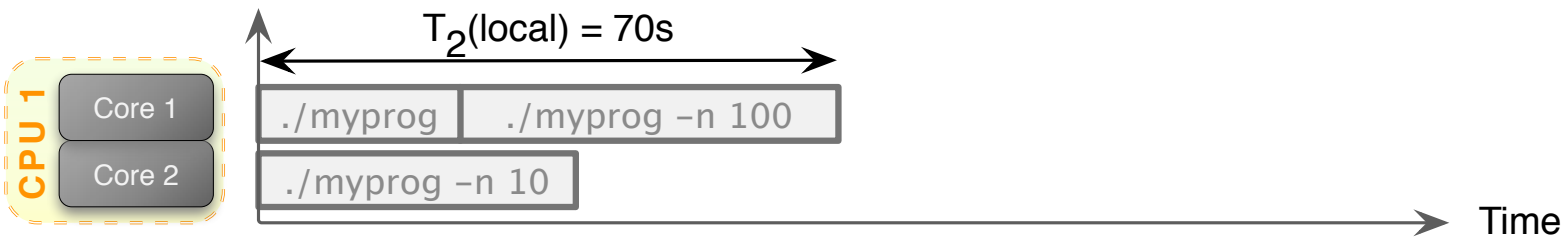

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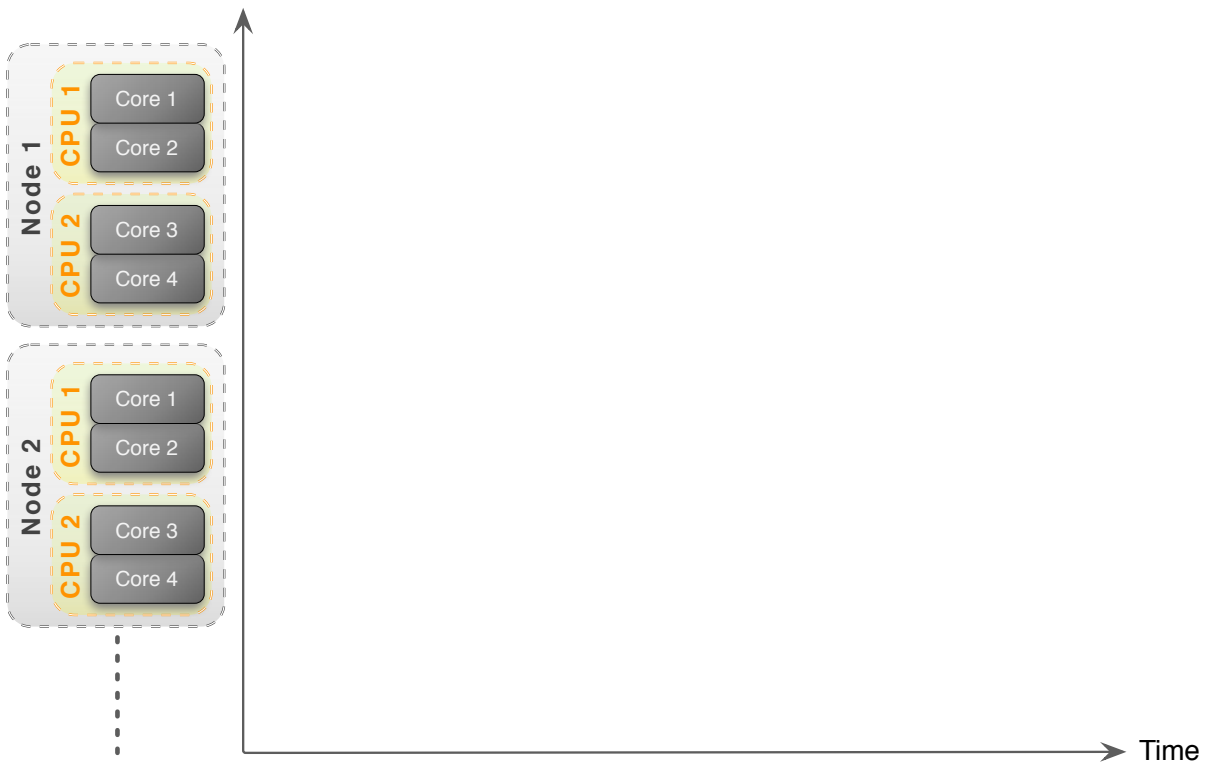

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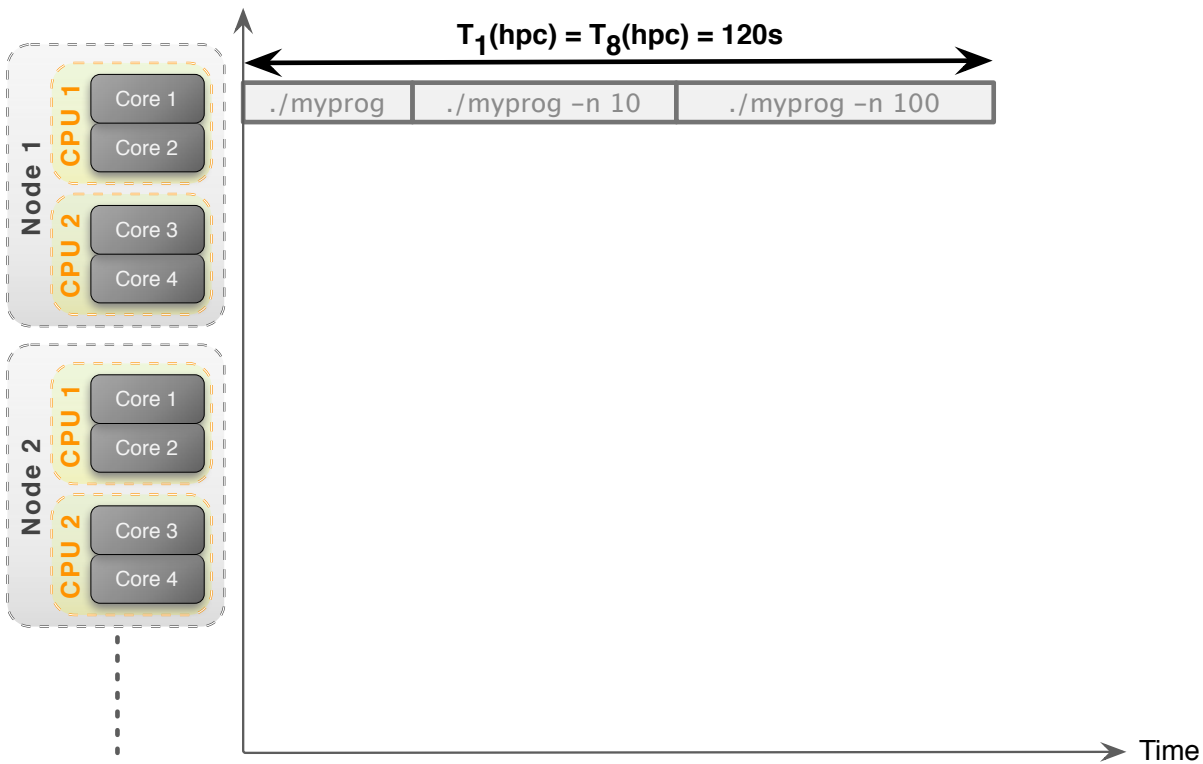

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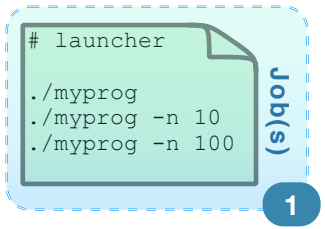

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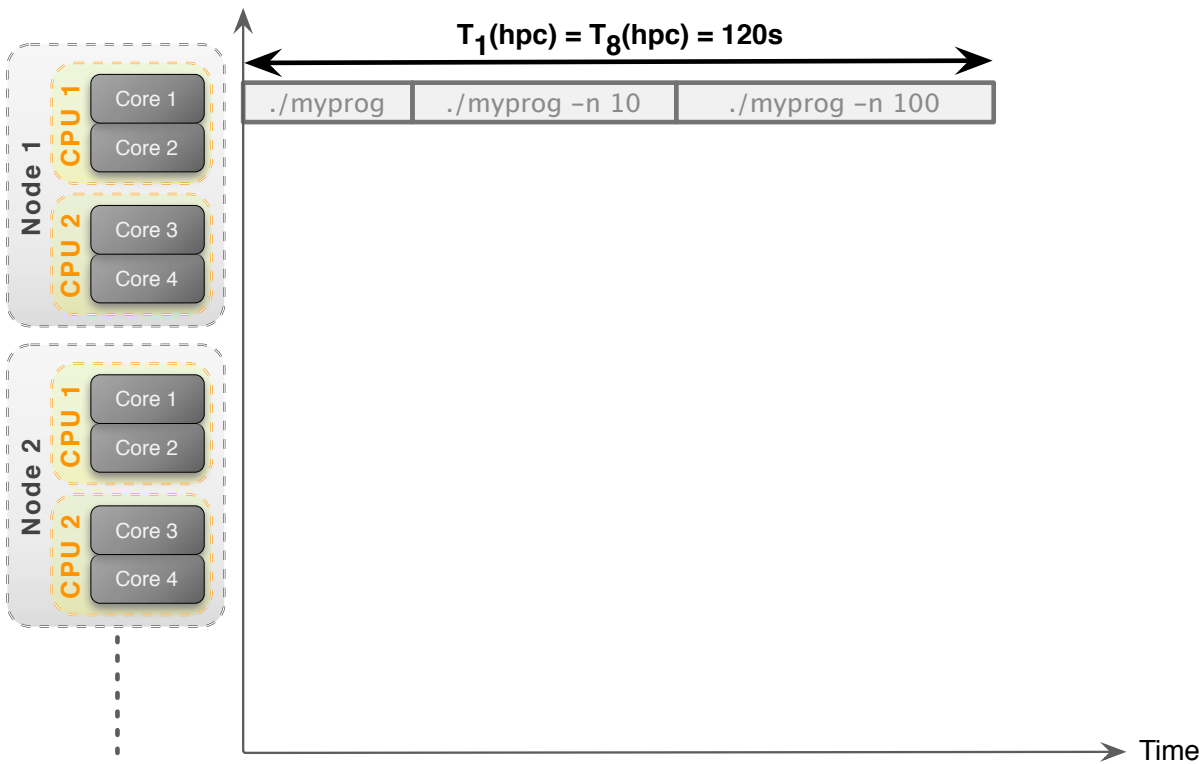

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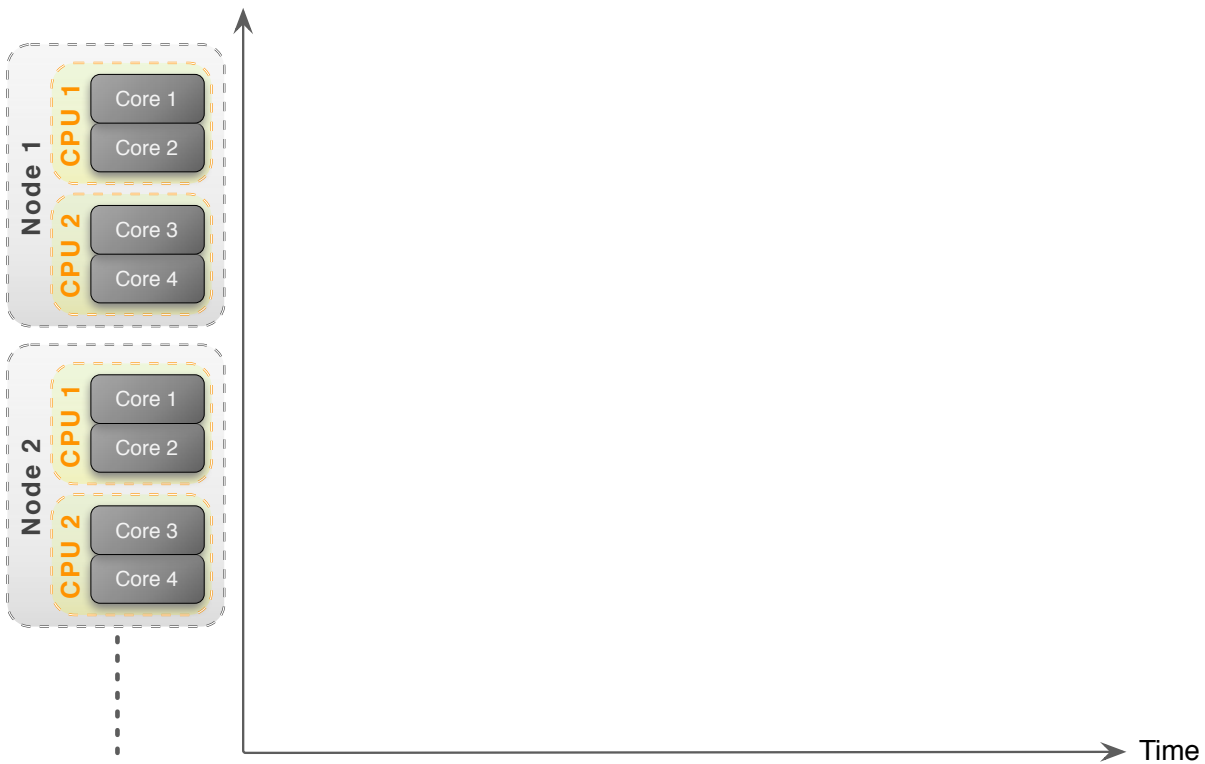

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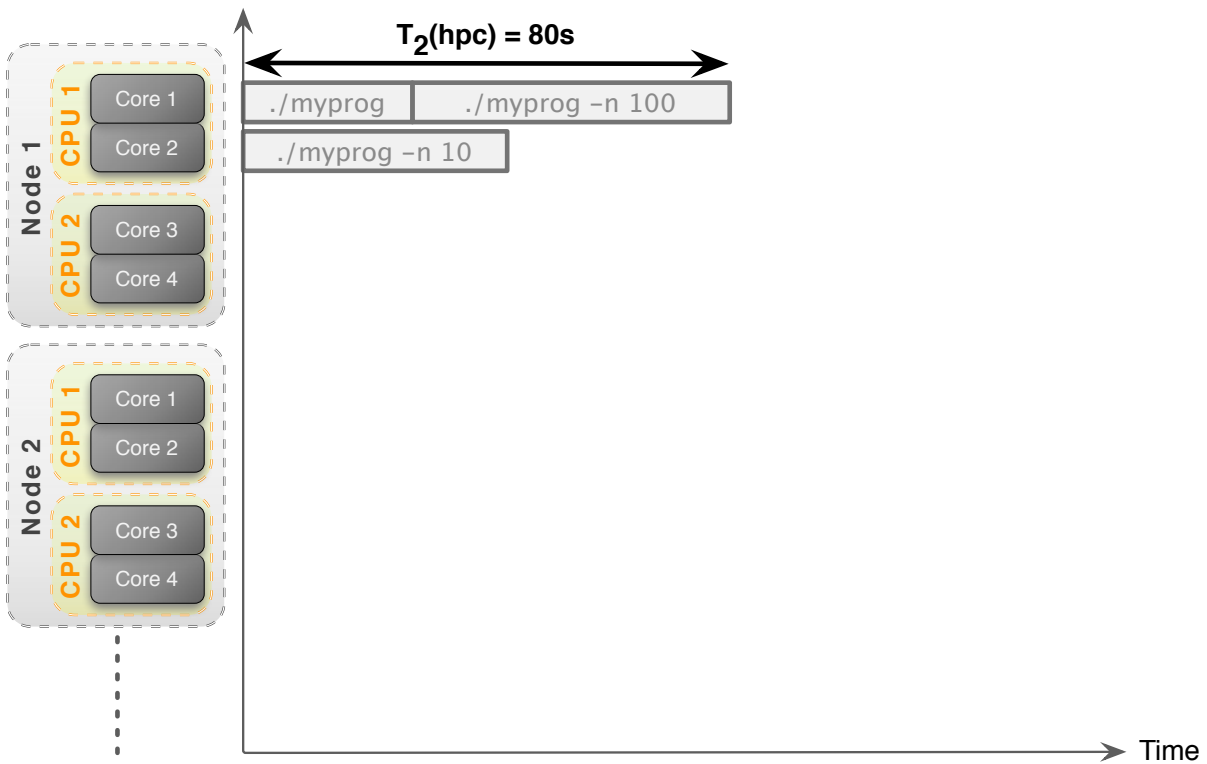

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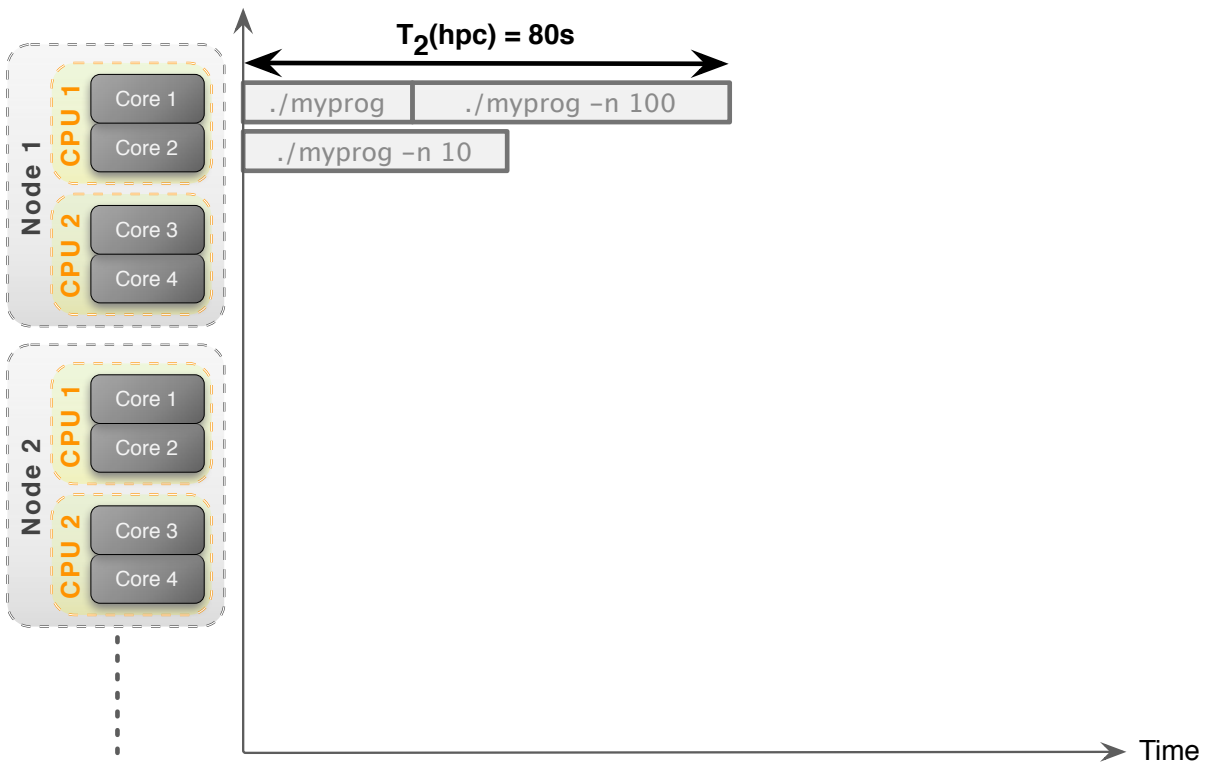

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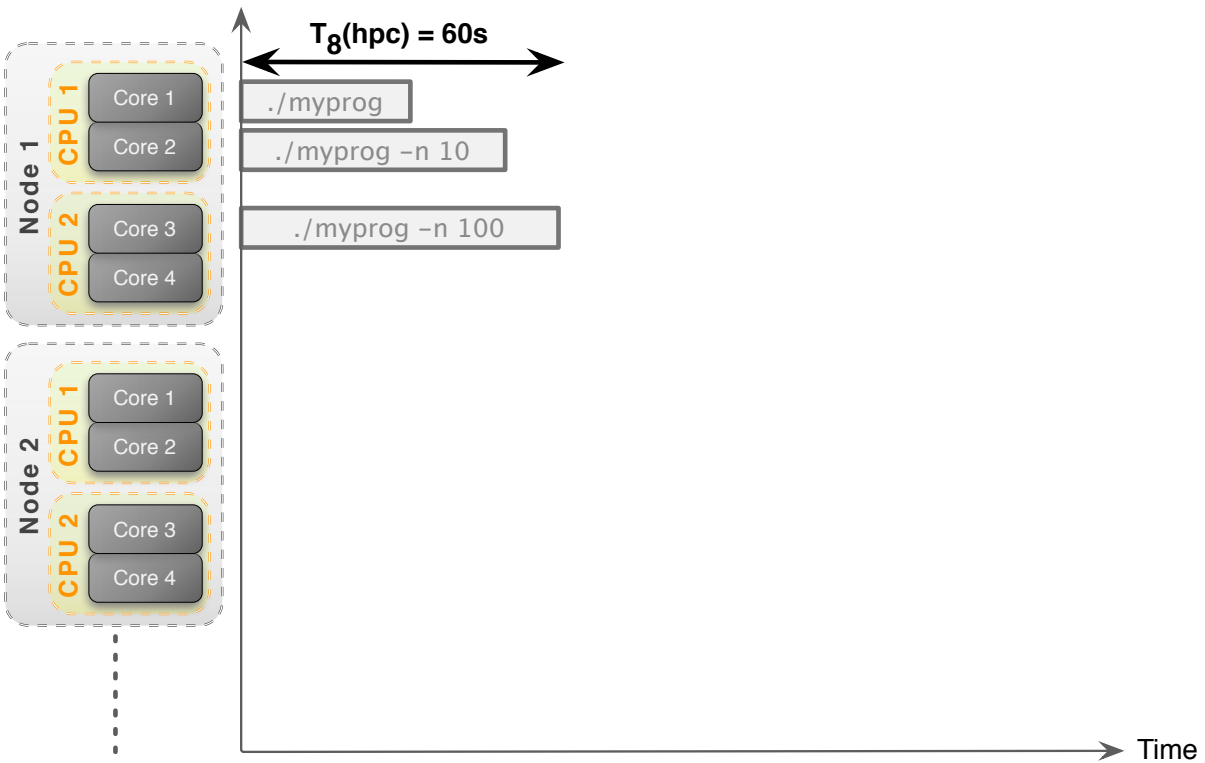

Local vs. HPC Executions

Context	Local PC	HPC
Sequential	$T_1(\text{local}) = 100\text{s}$	$T_1(\text{hpc}) = \mathbf{120s}$
Parallel/Distributed	$T_2(\text{local}) = 70\text{s}$	$T_2(\text{hpc}) = 80\text{s}$ $T_8(\text{hpc}) = 120\text{s}$ $T_8(\text{hpc}) = \mathbf{60s}$

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- **Sequential** runs **WON'T BE FASTER** on HPC
  - ↪ Reason: Processor Frequency (typically 3GHz vs 2.26GHz)

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- **Parallel/Distributed** runs **DO NOT COME FOR FREE**
  - ↪ runs **will be sequential** even if you reserve ≥ 2 cores/nodes
  - ↪ you have to **explicitly** adapt your jobs to benefit from the multi-cores/nodes

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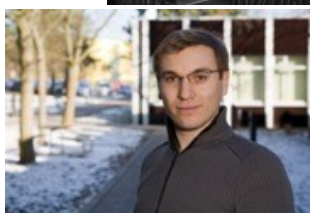
HPC @ UL

http://hpc.uni.lu

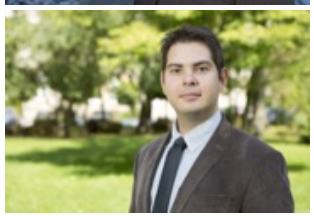
The UL HPC Team

Pascal Bouvry is a full professor of the FSTC and the head of the ILIAS research unit and the DS-CSCE doctoral school. His team (PCOG) is composed of 25 researchers working on Parallel computing and Optimization applied to Cloud Computing and HPC (scheduling, energy-efficiency, security), Ad-Hoc Networks (Vanets simulation and service optimization) and Biology (gene sequencing, regulatory networks, protein folding).

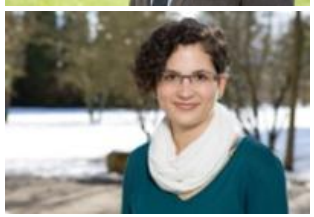
Sébastien Varrette, PhD, is a Research Associate in Prof. Bouvry's team since 2007. Along with Prof. Bouvry, he defined and set up the global HPC initiative of the UL in 2007. In this context, he is managing the sysadmin team that maintain and extend the platform. In parallel, his research work focuses on Distributed Computing Platforms (clusters, grids or clouds), with a particular interest on the security and performance evaluation of distributed or parallel executions.



Hyacinthe Cartiaux joined the HPC team in 2011 to set up the Grid'5000 Luxembourg site and has since been involved with all the HPC infrastructure of the UL, and other external services such as the Gforge. His interests cover IT automation and devops techniques, HPC & Grid Computing.

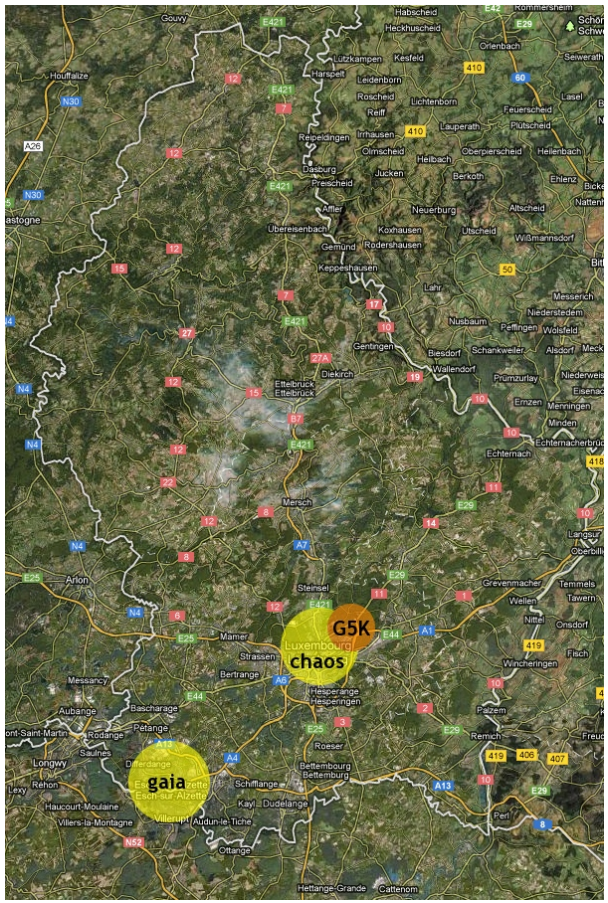


Valentin Plugaru is an HPC engineer part of the HPC team since 2014. Beginning with 2012 he has collaborated with Prof. Bouvry's team on research in Energy Efficiency and Performance Evaluation of HPC/Cloud environments. His general interests span R&D in High Performance Computing, Grid and Cloud Computing.



Sarah Diehl is a bioinformatician and joined the LCSB BioCore in 2015 as an HPC systems administrator. Her goal is to bridge the gap between researchers and IT specialists. She is experienced in data management, next-generation sequencing analysis and development of analysis pipelines.

UL HPC platforms at a glance (2015)



- **2 geographical sites**, **3 server rooms**
- **4 clusters**: `chaos+gaia`, `granduc`, `nyx`.
  - ↪ **400 nodes, 4284 cores, 49.918 TFlops**
  - ↪ incl. **18** dual [GP]GPU nodes
  - ↪ **4268.4 TB (raw) shared storage**
    - ✓ incl. 1.5 PB for backup
    - ✓ incl. **1.4 PB** (EMC Isilon) SIU/LCSB/HPC
- **4 sysadmins** `hpc-sysadmins@uni.lu`
- **6,340,316€ (Cumul. HW Investment)** since 2007
  - ↪ Hardware acquisition only
  - ↪ 4,077,913€ (excluding server rooms)
- **Open-Source** software stack
  - ↪ SSH, LDAP, OAR, Puppet, Modules...

HPC server rooms

- **2009** CS.43 (Kirchberg campus) 14 racks, 100 m^2, $\simeq$ 800,000€



- **2011** LCSB 6^{th} floor (Belval) 14 racks, 112 m^2, $\simeq$ 1,100,000€

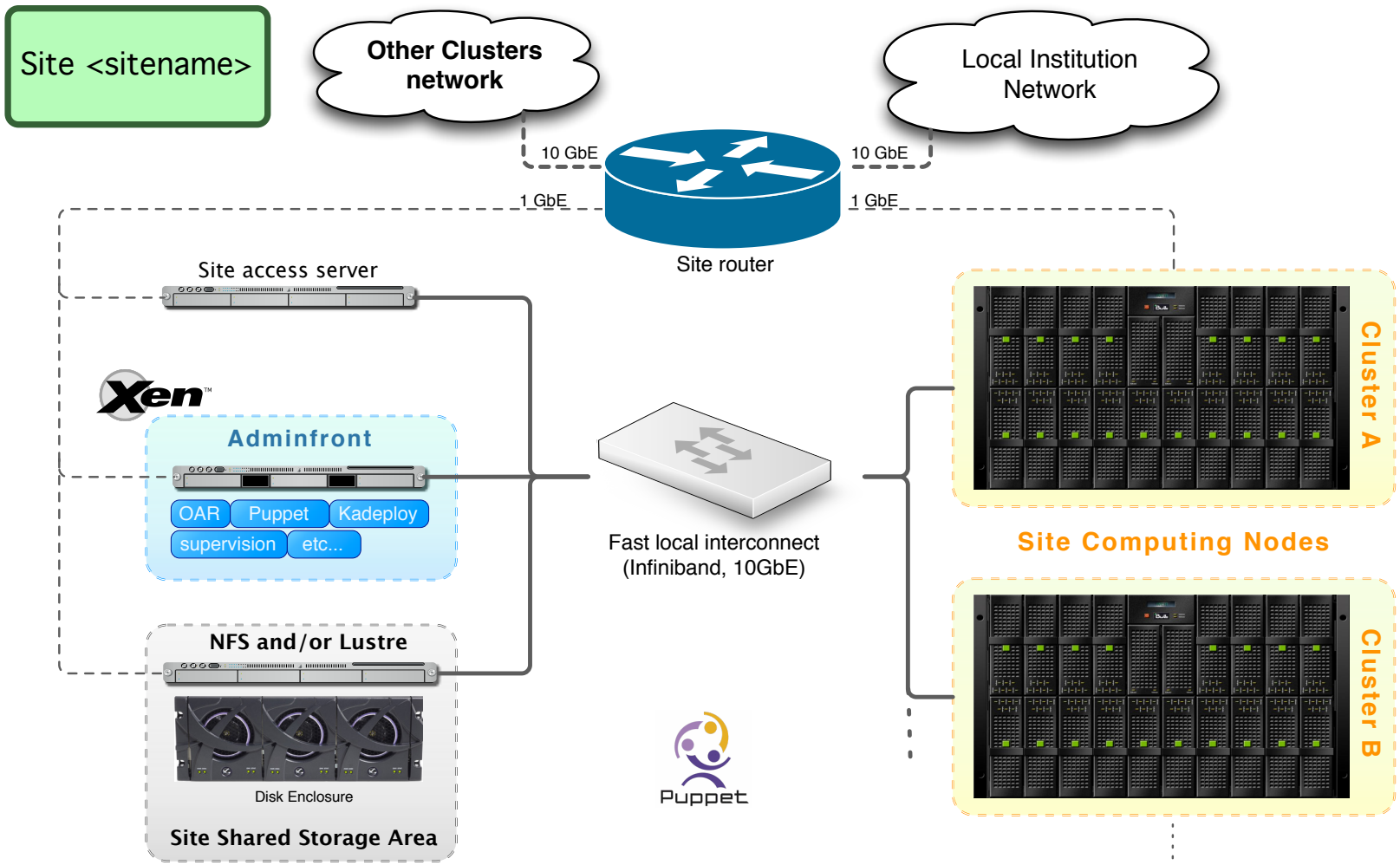

UL HPC Computing Nodes

	Date	Vendor	Proc. Description		#N	#C	R_{peak}
chaos	2010	HP	Intel Xeon L5640@2.26GHz	2 × 6C,24GB	32	384	3.472 TFlops
	2011	Dell	Intel Xeon L5640@2.26GHz	2 × 6C,24GB	16	192	1.736 TFlops
	2012	Dell	Intel Xeon X7560@2,26GHz	4 × 6C, 1TB	1	32	0.289 TFlops
	2012	Dell	Intel Xeon E5-2660@2.2GHz	2 × 8C,32GB	16	256	4.506 TFlops
	2012	HP	Intel Xeon E5-2660@2.2GHz	2 × 8C,32GB	16	256	4.506 TFlops
				`chaos` **TOTAL:**	**81**	**1120**	**14.509 TFlops**
gaia	2011	Bull	Intel Xeon L5640@2.26GHz	2 × 6C,48GB	72	864	7.811 TFlops
	2012	Dell	Intel Xeon E5-4640@2.4GHz	4 × 8C, 1TB	1	32	0.307 TFlops
	2012	Bull	Intel Xeon E7-4850@2GHz	16 × 10C,1TB	1	160	1.280 TFLops
	2013	Dell	Intel Xeon E5-2660@2.2GHz	2 × 8C,64GB	5	80	1.408 TFlops
	2013	Bull	Intel Xeon X5670@2.93GHz	2 × 6C,48GB	40	480	5.626 TFlops
	2013	Bull	Intel Xeon X5675@3.07GHz	2 × 6C,48GB	32	384	4.746 TFlops
	2014	Delta	Intel Xeon E78880@2.5 GHz	8 × 15C,1TB	1	120	2.4 TFlops
	2014	SGi	Intel Xeon E54650@2.4 GHz	16 × 10C,4TB	1	160	3.072 TFlops
				`gaia` **TOTAL:**	**153**	**2280**	**26.96 TFlops**
g5k	2008	Dell	Intel Xeon L5335@2GHz	2 × 4C,16GB	22	176	1.408 TFlops
	2012	Dell	Intel Xeon E5-2630L@2GHz	2 × 6C,24GB	16	192	3.072 TFlops
				`granduc/petitprince` **TOTAL:**	**38**	**368**	**4.48 TFlops**

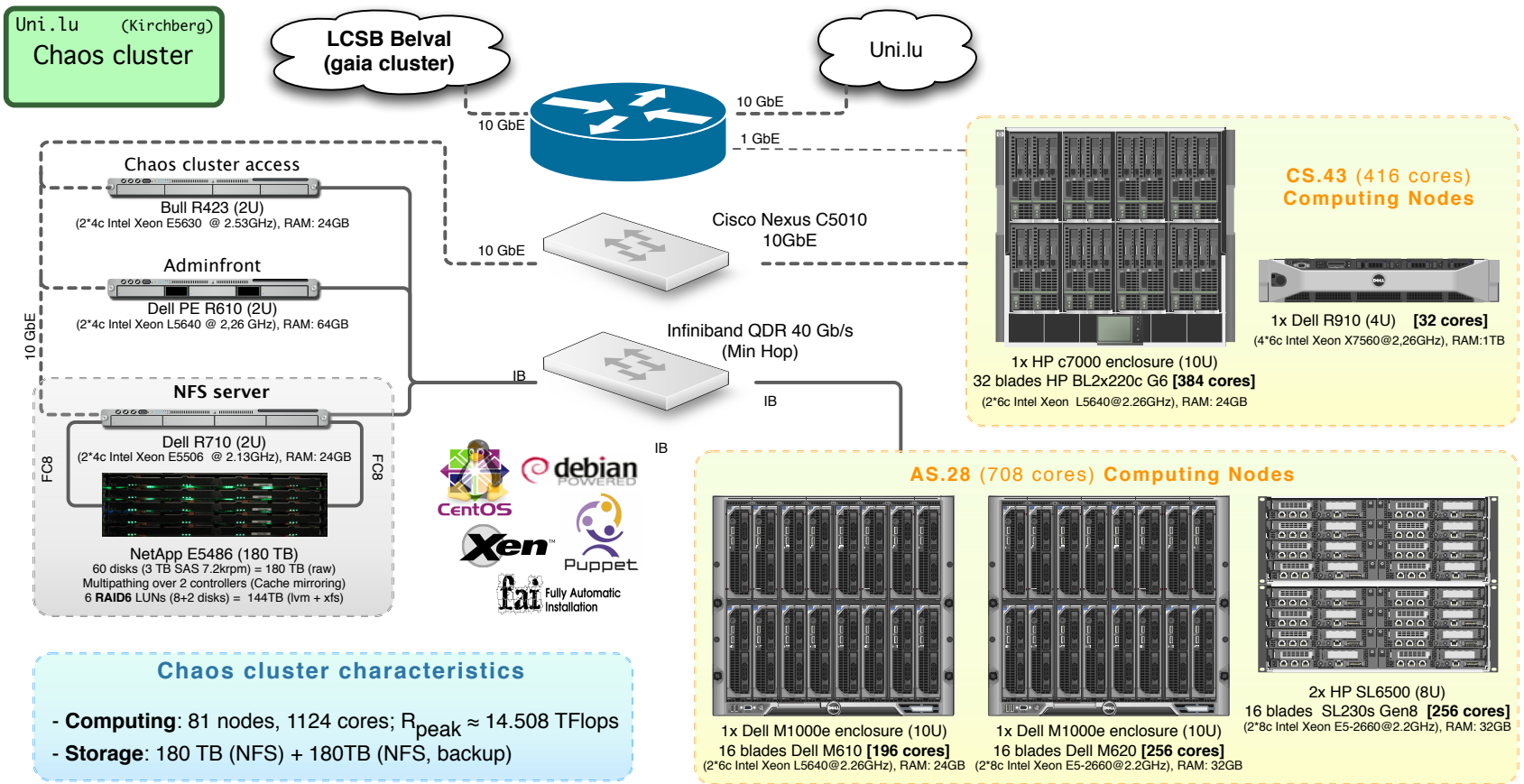
Testing cluster:

nyx	2012	Dell	Intel Xeon E5-2420@1.9GHz	1 × 6C,32GB	2	12	0.091 TFlops
	2013	Viridis	ARM A9 Cortex@1.1GHz	1 × 4C,4GB	96	384	0.422 TFlops
	2015	HP	Intel E3-1284Lv3, 1.8GHz	1 × 4C,32GB	30	120	3.456 TFlops
				`nyx/viridis` **TOTAL:**	**128**	**516**	**3.969 TFlops**

UL HPC: General cluster organization



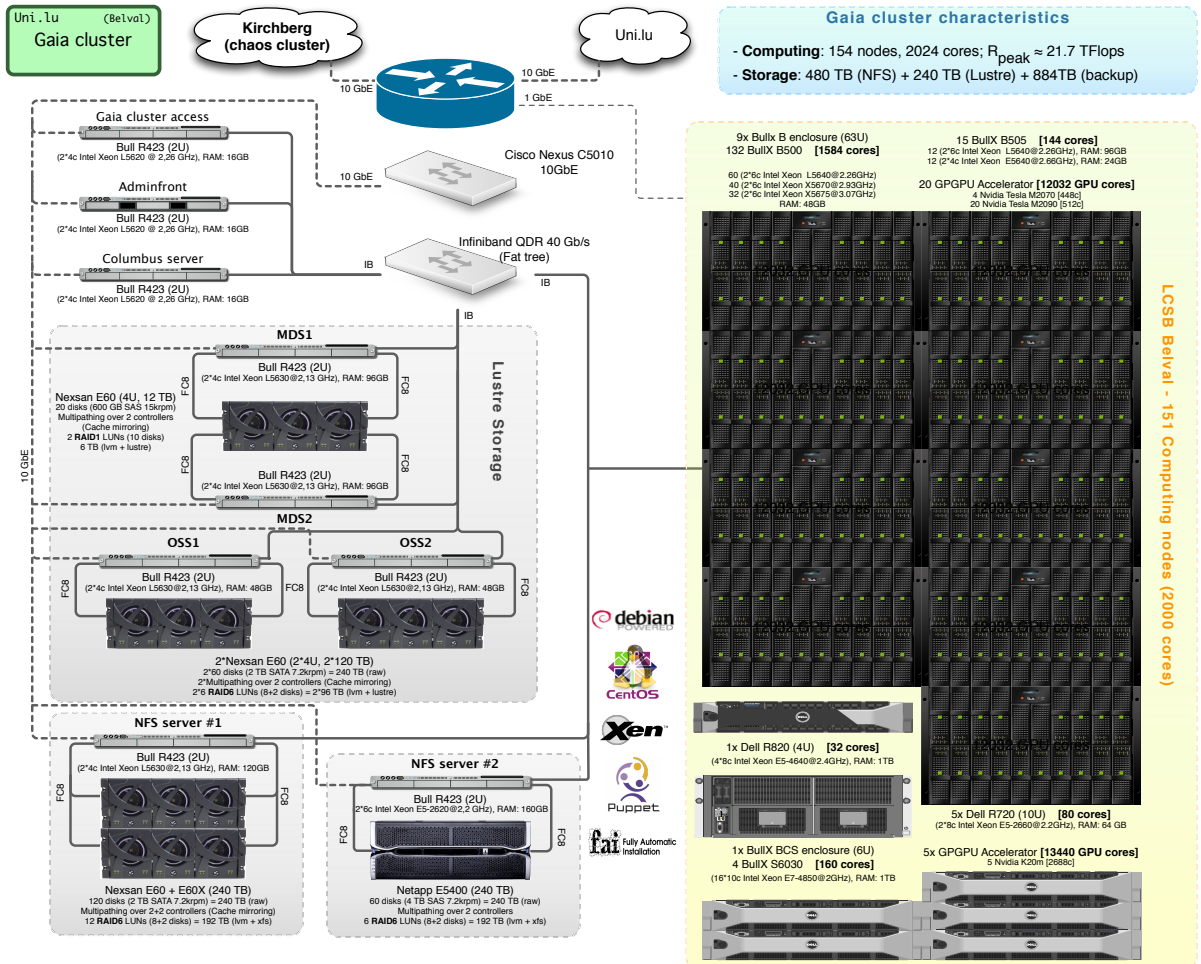
Ex: The chaos cluster



Chaos cluster characteristics

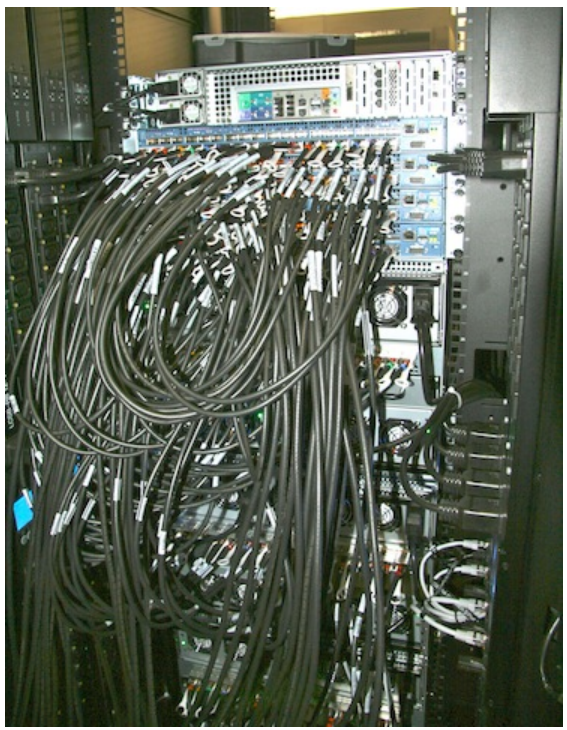
- **Computing**: 81 nodes, 1124 cores; $R_{peak} \approx 14.508$ TFlops
- **Storage**: 180 TB (NFS) + 180TB (NFS, backup)

Ex: The gaia cluster



Ex: Some racks of the gaia cluster





UL HPC Software Stack

- **Operating System:** Linux Debian (CentOS on storage servers)
- **Remote connection to the platform**: SSH
- **User SSO**: OpenLDAP-based
- **Resource management**: job/batch scheduler: OAR
- **(Automatic) Computing Node Deployment**:
  - ↪ FAI (Fully Automatic Installation) (`chaos,gaia,nyx` only)
  - ↪ Puppet
  - ↪ Kadeploy (`granduc,petitprince`/Grid5000 only)
- **Platform Monitoring**: OAR Monika, OAR Drawgantt, Ganglia, Nagios, Puppet Dashboard etc.
- **Commercial Softwares**:
  - ↪ Intel Cluster Studio XE, TotalView, Allinea DDT, Stata etc.

HPC in the Grande region and Around

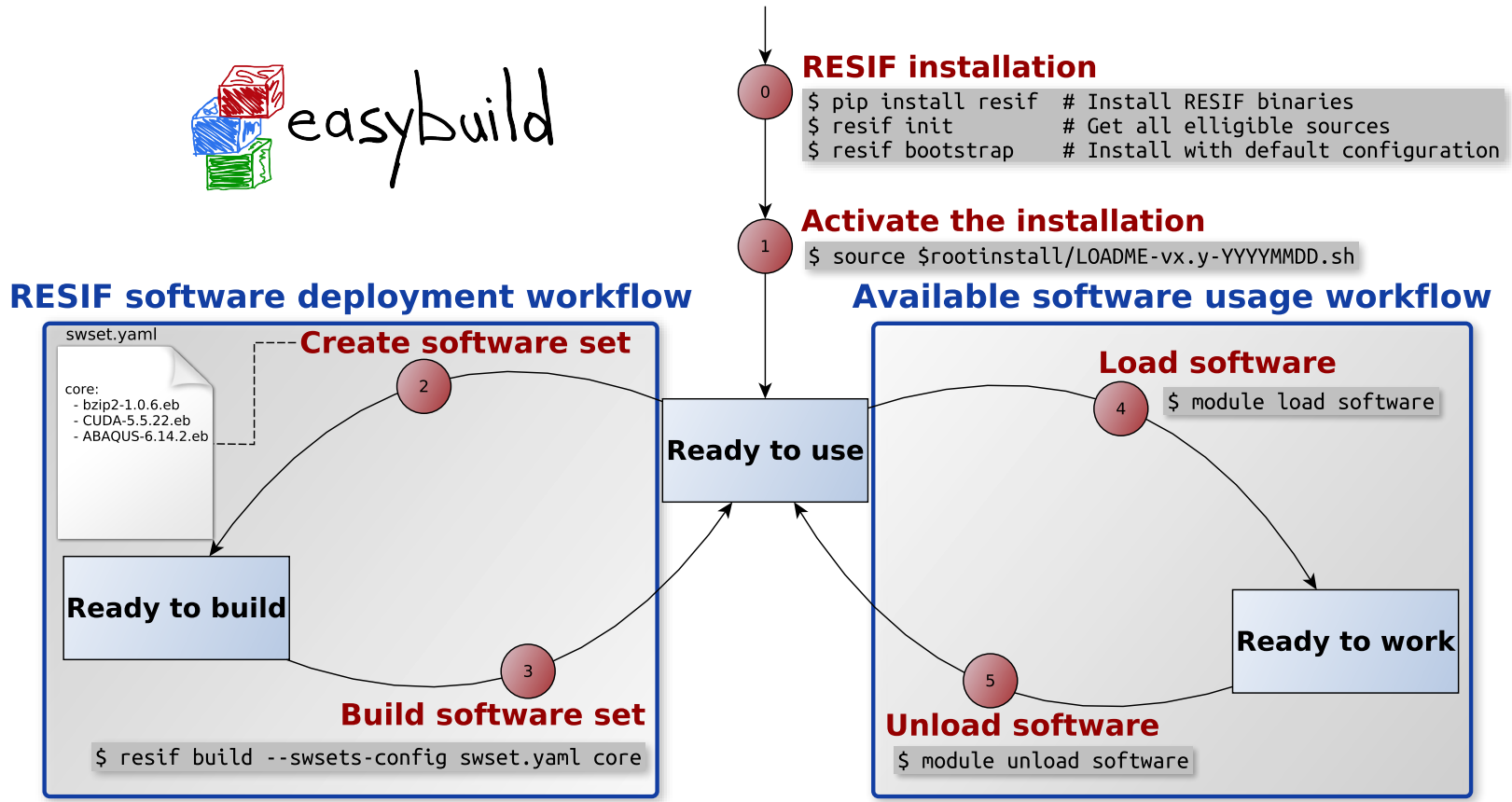
			TFlops	TB	FTEs
Country	**Name/Institute**	**#Cores**	**R_{peak}**	**Storage**	**Manpower**
Luxembourg	UL	4284	49.918	4268.4	4
	CRP GL	800	6.21	144	1.5
France	TGCC Curie, CEA	77184	1667.2	5000	n/a
	LORIA, Nancy	3724	29.79	82	5.05
	ROMEO (GPU*), Reims	5720	254,9 TFlops*	245	2
Germany	Juqueen, Juelich	393216	5033.2	448	n/a
	MPI, RZG	2556	14.1	n/a	5
	URZ, (bwGrid),Heidelberg	1140	10.125	32	9
Belgium	UGent, VCS	4320	54.541	82	n/a
	CECI, UMons/UCL	2576	25.108	156	> 4
UK	Darwin, Cambridge Univ	9728	202.3	20	n/a
	Legion, UCLondon	5632	45.056	192	6
Spain	MareNostrum, BCS	33664	700.2	1900	14

Software/Modules Management

- RESIF: Revolutionary EasyBuild-based Software Installation Framework
  - ↪ Automatic Management of Environment Modules deployment
  - ↪ Fully automates software builds and supports all available toolchains
  - ↪ Clean (hierarchical) modules layout to facilitate its usage
  - ↪ "Easy to use"
- Cf Tutorials: http://ulhpc-tutorials.readthedocs.org/

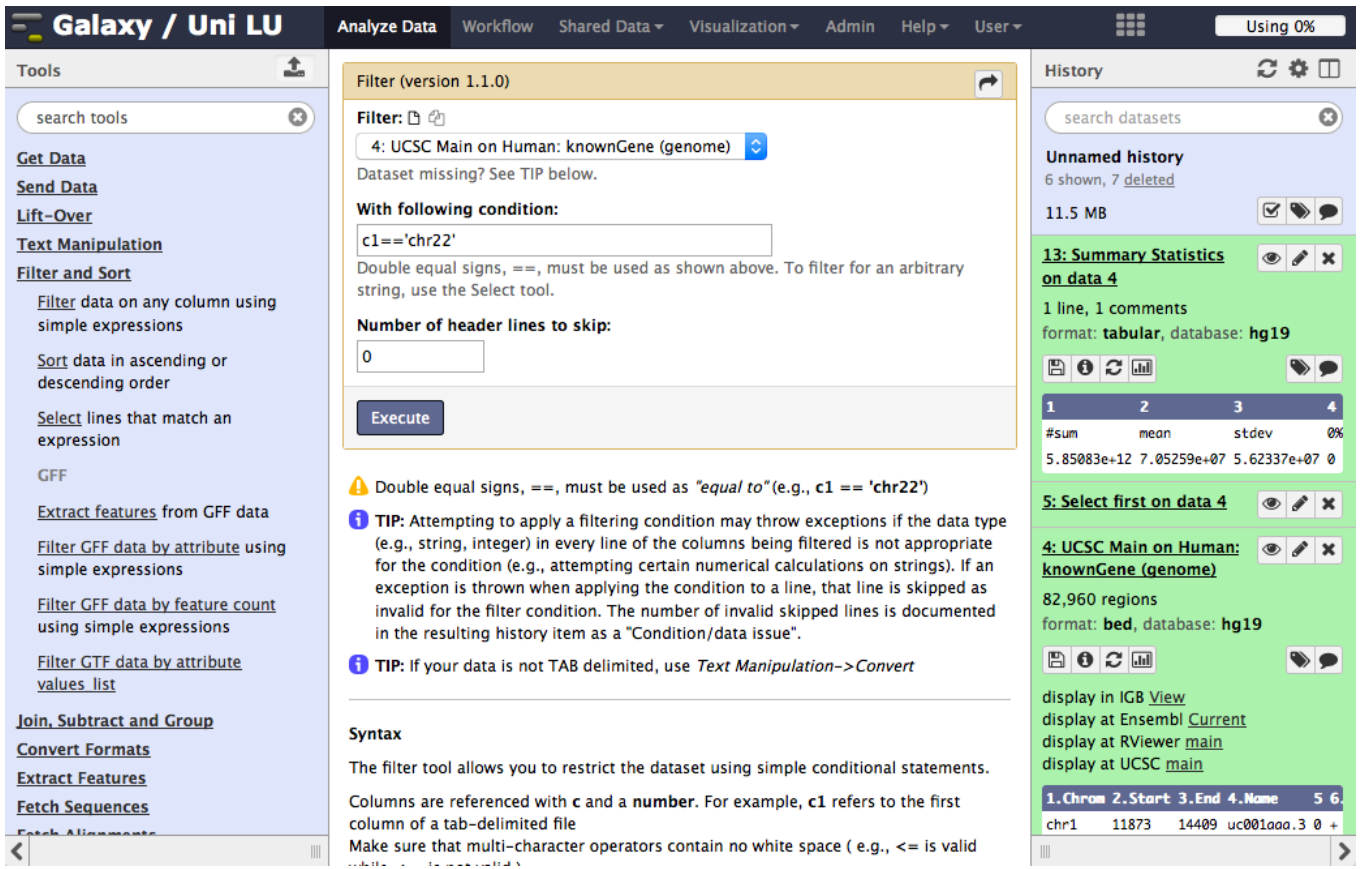
Software/Modules Management

RESIF: Revolutionary EasyBuild-based Software Installation Framework



BIO Workflow Management

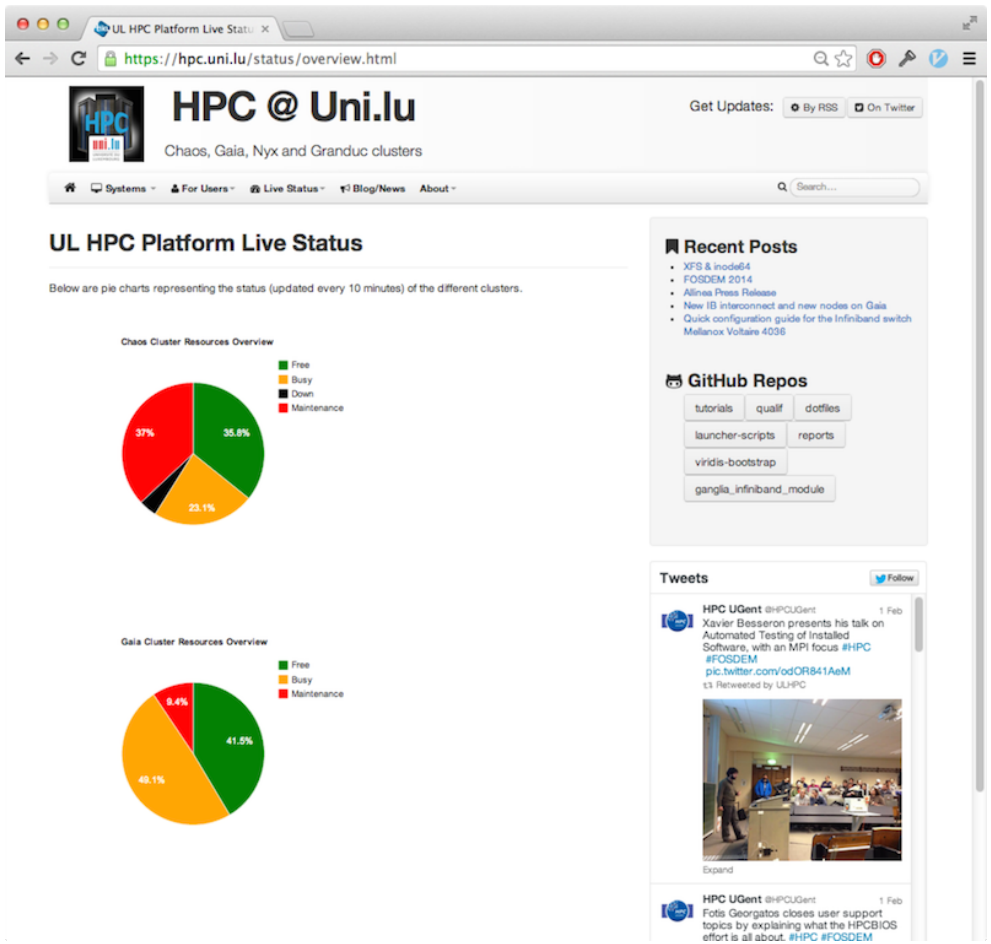
- Galaxy Portal `galaxy-server.uni.lu`
  - ↪ web-based platform for data intensive biomedical research.



Platform Monitoring

General Live Status

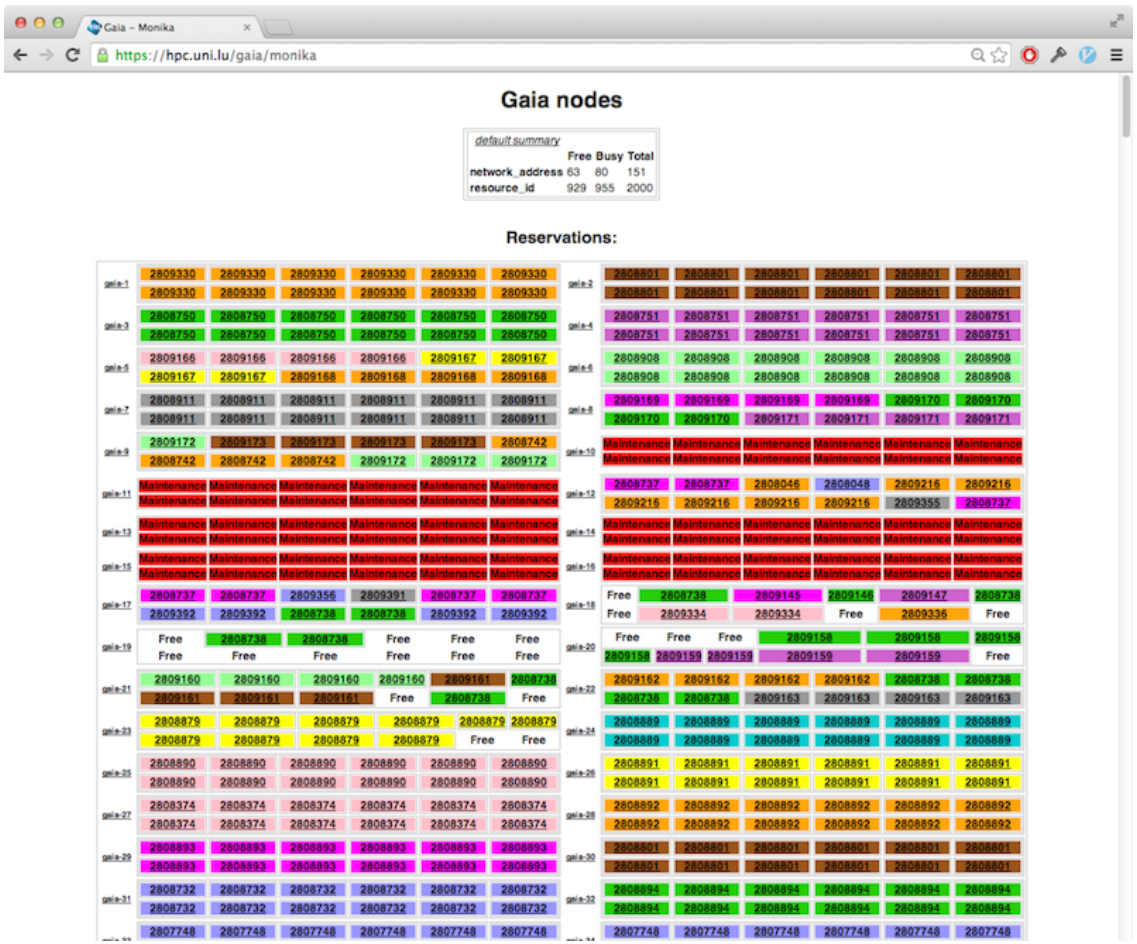
http://hpc.uni.lu/status/overview.html



Platform Monitoring

Monika

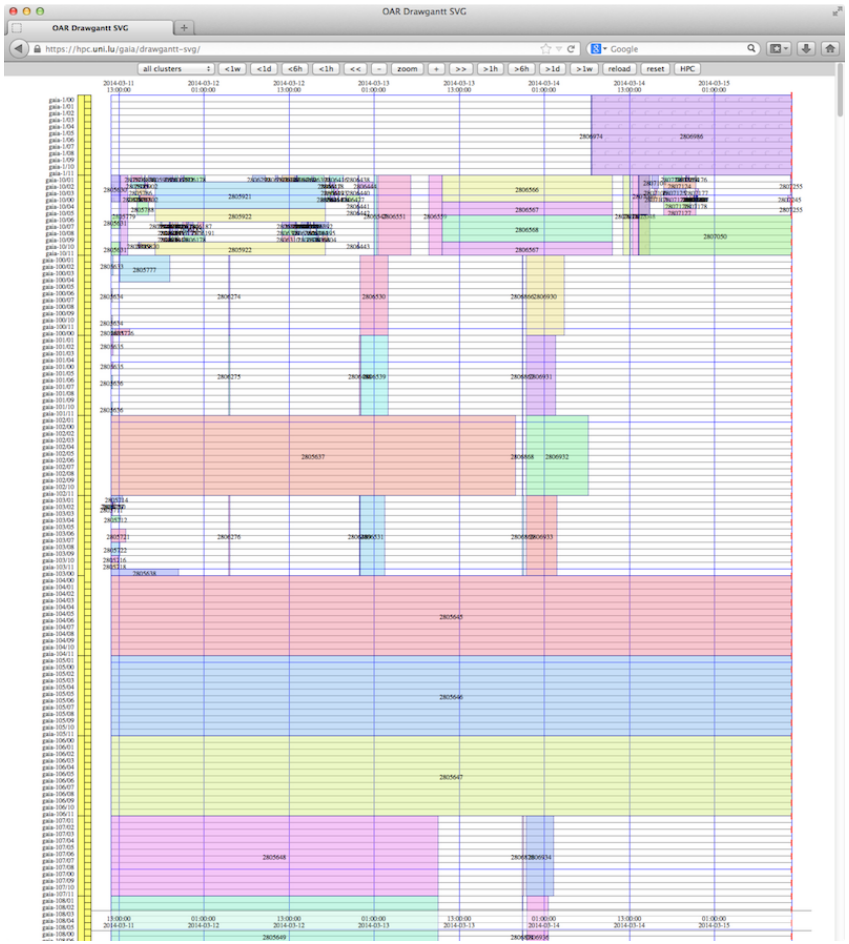
http://hpc.uni.lu/{chaos,gaia,g5k}/monika



Platform Monitoring

Drawgantt

http://hpc.uni.lu/{chaos,gaia,g5k}/drawgantt



Platform Monitoring

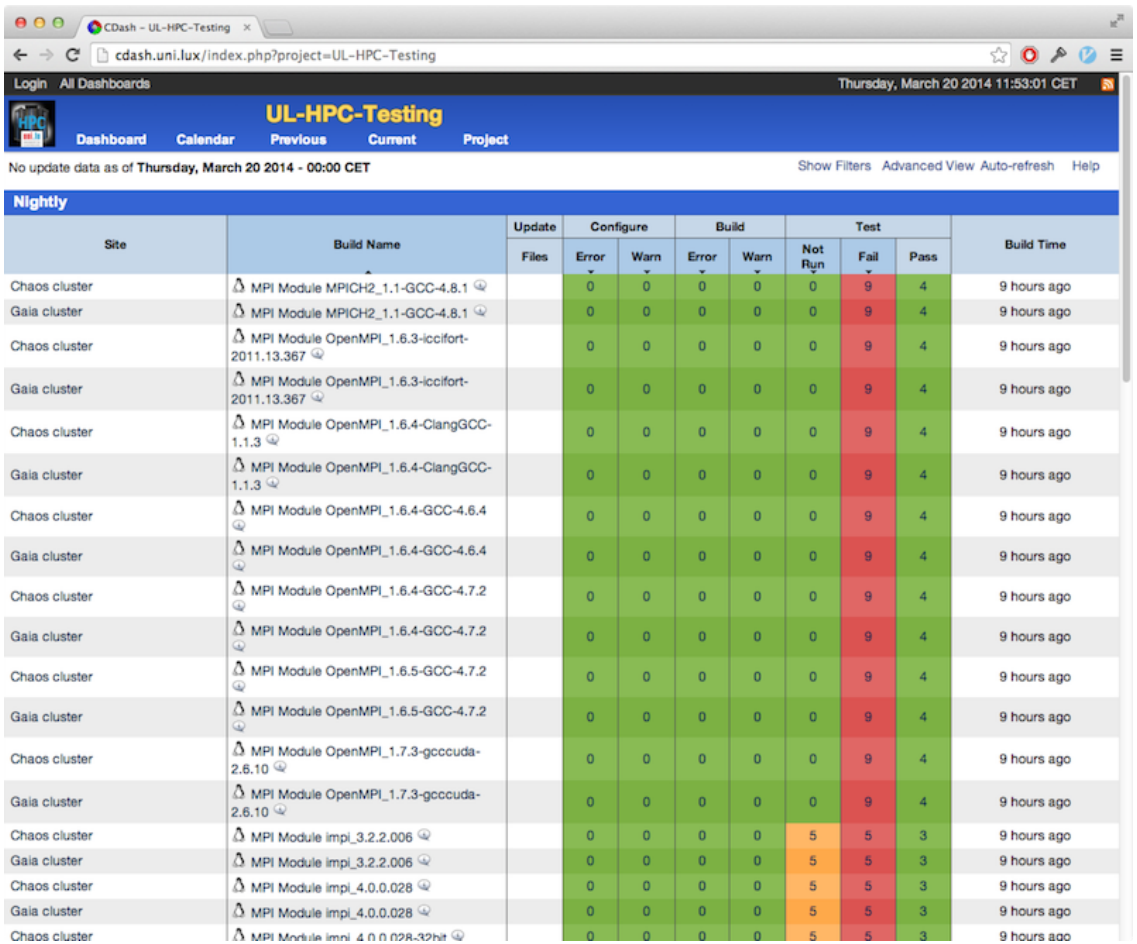
Ganglia

http://hpc.uni.lu/{chaos,gaia,g5k}/ganglia

Platform Monitoring

CDash

http://cdash.uni.lu/



CDash - UL-HPC-Testing

cdash.uni.lux/index.php?project=UL-HPC-Testing

Login All Dashboards Thursday, March 20 2014 11:53:01 CET

UL-HPC-Testing

Dashboard Calendar Previous Current Project

No update data as of **Thursday, March 20 2014 - 00:00 CET**

Show Filters Advanced View Auto-refresh Help

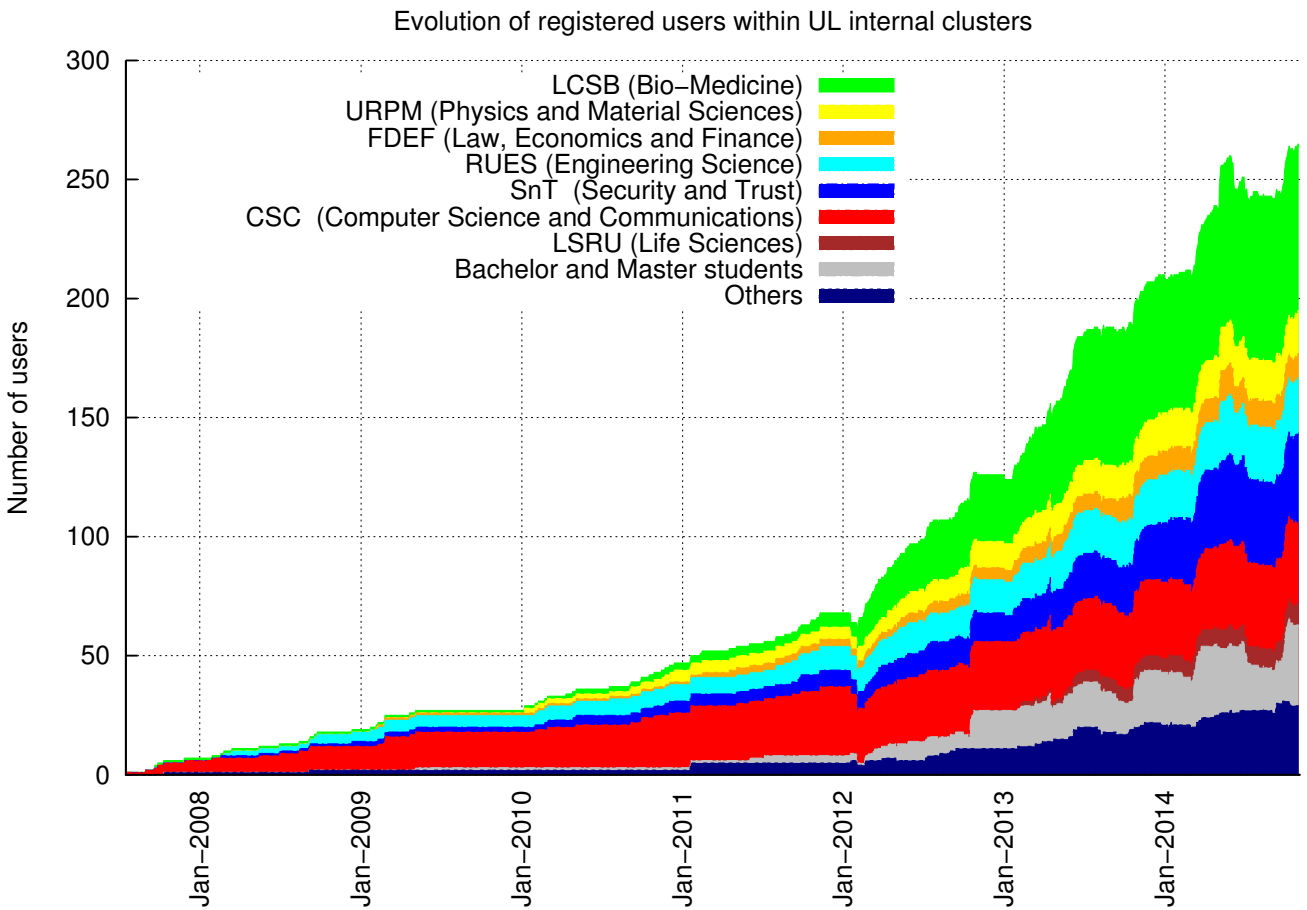
Nightly

Site	Build Name	Update	Configure		Build		Test			Build Time
		Files	Error	Warn	Error	Warn	Not Run	Fail	Pass	
Chaos cluster	MPI Module MPICH2_1.1-GCC-4.8.1		0	0	0	0	0	9	4	9 hours ago
Gaia cluster	MPI Module MPICH2_1.1-GCC-4.8.1		0	0	0	0	0	9	4	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.6.3-iccifort-2011.13.367		0	0	0	0	0	9	4	9 hours ago
Gaia cluster	MPI Module OpenMPI_1.6.3-iccifort-2011.13.367		0	0	0	0	0	9	4	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.6.4-ClangGCC-1.1.3		0	0	0	0	0	9	4	9 hours ago
Gaia cluster	MPI Module OpenMPI_1.6.4-ClangGCC-1.1.3		0	0	0	0	0	9	4	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.6.4-GCC-4.6.4		0	0	0	0	0	9	4	9 hours ago
Gaia cluster	MPI Module OpenMPI_1.6.4-GCC-4.6.4		0	0	0	0	0	9	4	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.6.4-GCC-4.7.2		0	0	0	0	0	9	4	9 hours ago
Gaia cluster	MPI Module OpenMPI_1.6.4-GCC-4.7.2		0	0	0	0	0	9	4	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.6.5-GCC-4.7.2		0	0	0	0	0	9	4	9 hours ago
Gaia cluster	MPI Module OpenMPI_1.6.5-GCC-4.7.2		0	0	0	0	0	9	4	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.7.3-gcccuda-2.6.10		0	0	0	0	0	9	4	9 hours ago
Gaia cluster	MPI Module OpenMPI_1.7.3-gcccuda-2.6.10		0	0	0	0	0	9	4	9 hours ago
Chaos cluster	MPI Module impi_3.2.2.006		0	0	0	0	5	5	3	9 hours ago
Gaia cluster	MPI Module impi_3.2.2.006		0	0	0	0	5	5	3	9 hours ago
Chaos cluster	MPI Module impi_4.0.0.028		0	0	0	0	5	5	3	9 hours ago
Gaia cluster	MPI Module impi_4.0.0.028		0	0	0	0	5	5	3	9 hours ago
Chaos cluster	MPI Module impi_4.0.0.028-32bit		0	0	0	0	5	5	3	9 hours ago

UL HPC Key numbers Summary

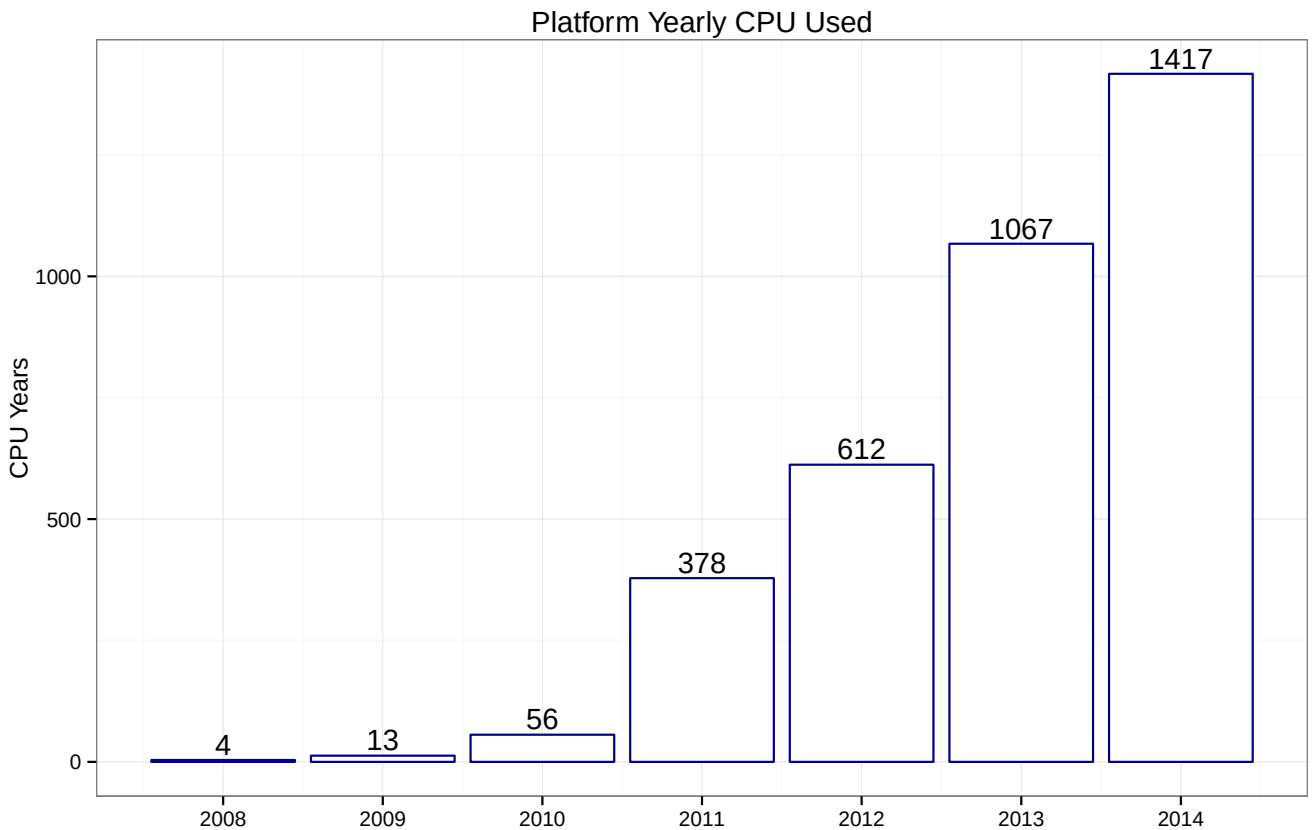
- **400 nodes, 4284 cores, 49.918 TFlops**
  - ↪ Mostly Intel-based architecture
  - ↪ multi vendors (Bull, HP, Dell, Delta, SGi)
- **4268.4 TB shared storage**
  - ↪ Based on NetApp / NexSAN / Certon disk enclosures
  - ↪ **Homedirs** / **Projects**: NFS, GPFS, OneFS — 2.36 PB
  - ↪ **Scratch** Lustre — 0.48 PB
  - ↪ **Backup**: NFS, GlusterFS — 1.4 PB
- **6,340,316€ (Cumul. HW Investment)** — since 2007
- 281 registered users

Registered Users

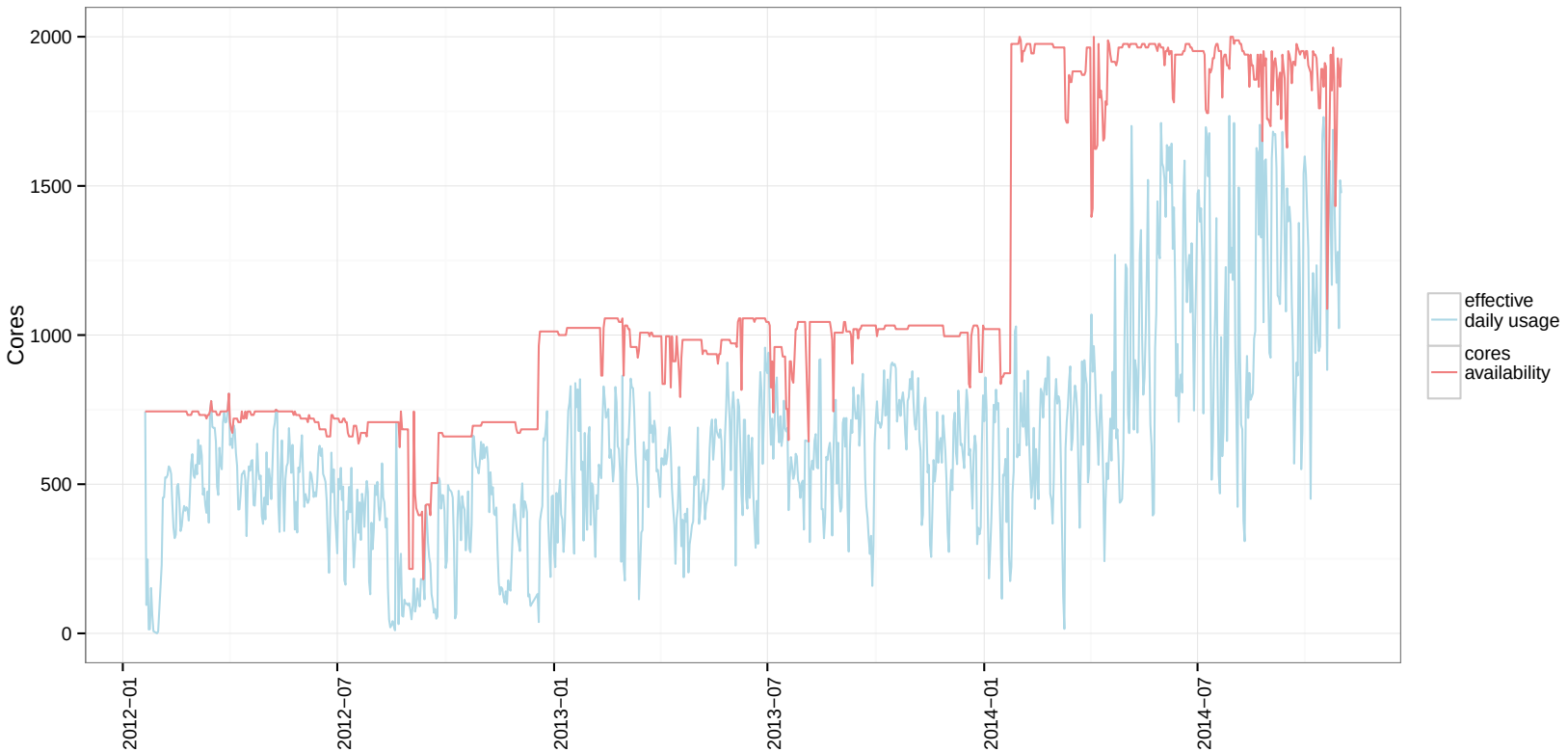


CPU-year usage since 2008

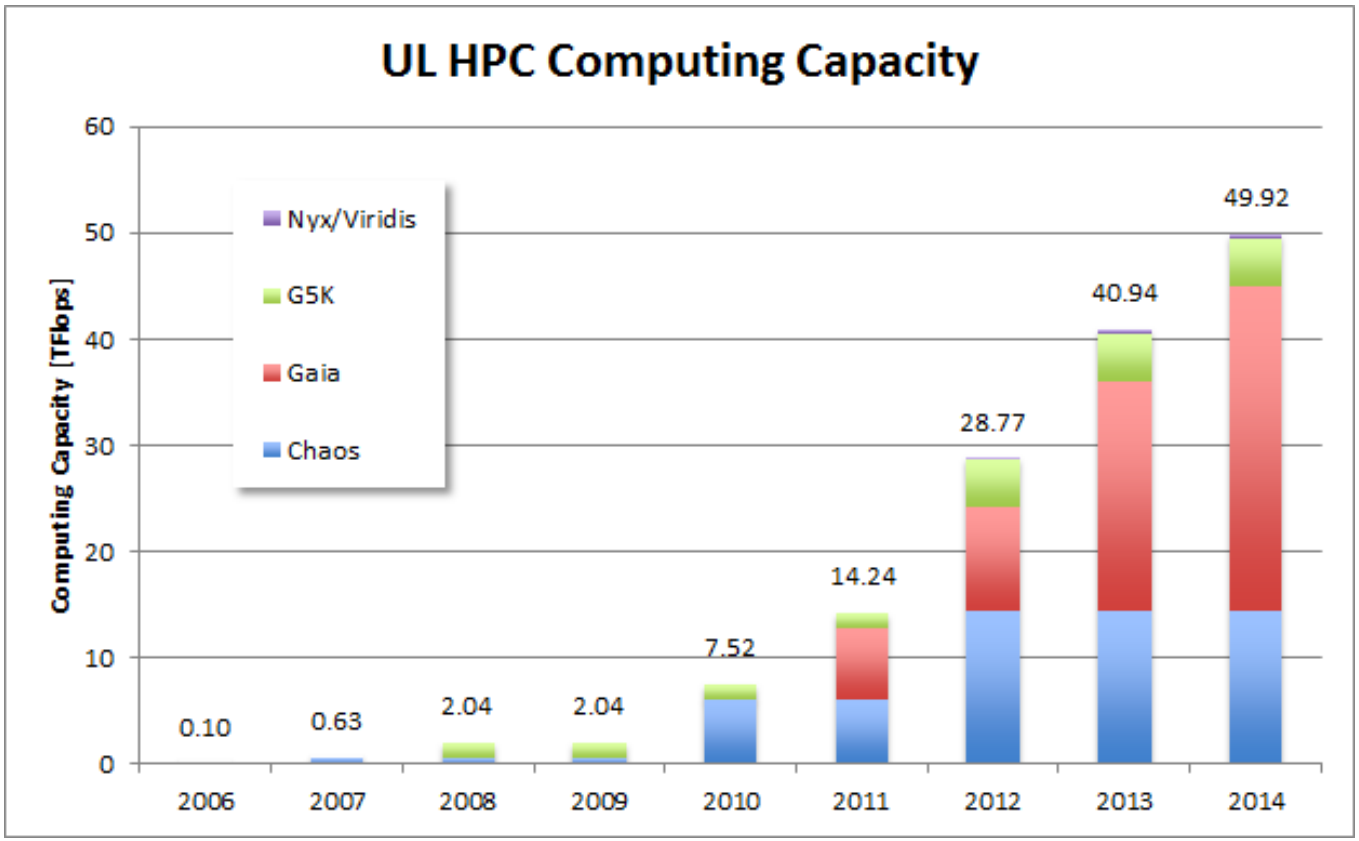
- **CPU-hour**: *work* done by a CPU in one hour of wall clock time



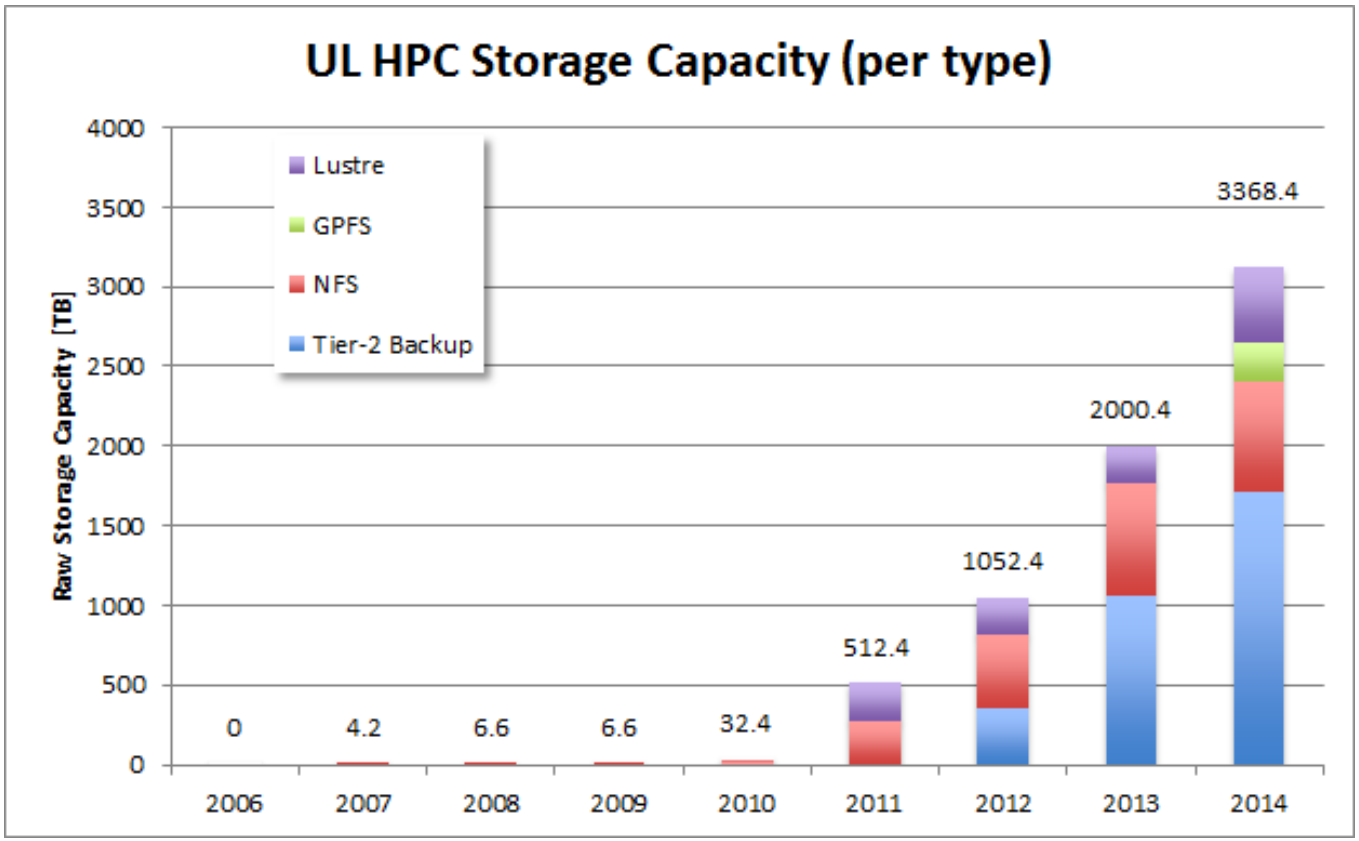
A Year on Gaia...



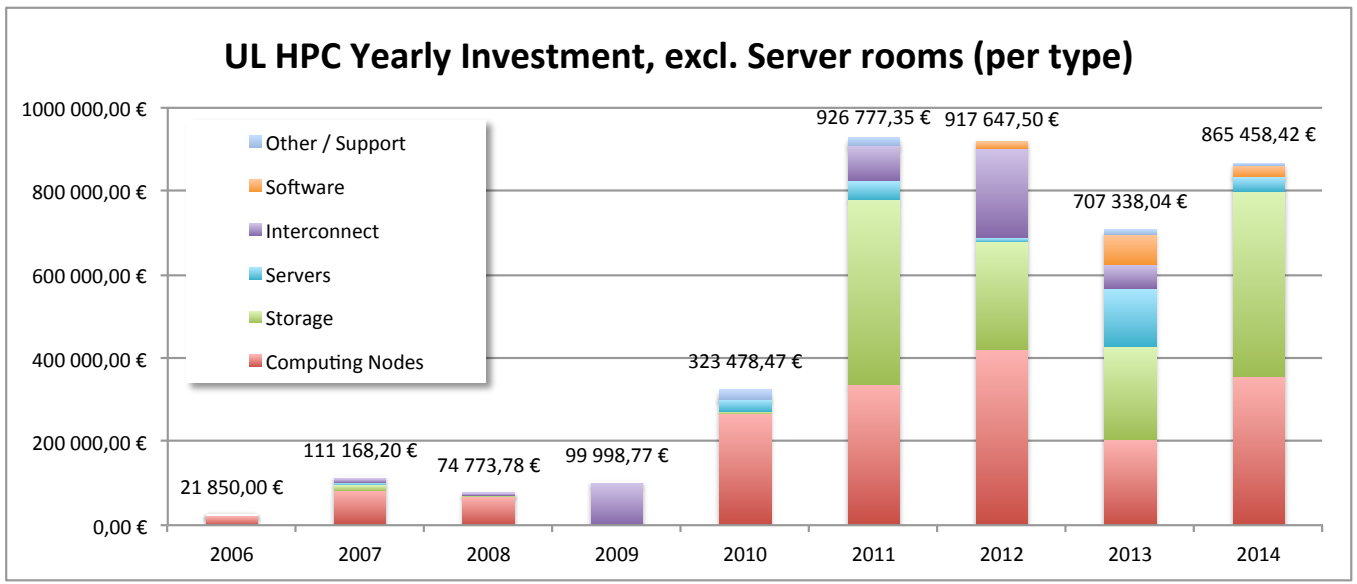
Chronological Statistics



Chronological Statistics



Chronological Statistics



Research Domains and Usage

Research Domains (Among the 288 registered users)

- **Research Areas** that currently benefit from UL HPC platforms:
  - ↪ Security ([Ad-Hoc] Network, FT, Grid, Cloud etc.)
  - ↪ Mechanical Engineering
  - ↪ Physics, Geo-Physics
  - ↪ [Multi-Objective] Optimization [Robust] Task Scheduling etc.
  - ↪ Cryptology
  - ↪ Economy
  - ↪ Life Sciences

Summary

1 Preliminaries

2 The UL HPC platform
Overview
Platform Management Tools
Monitoring
Statistics & Milestones

3 Incoming Milestones and Challenges

2015 Milestones

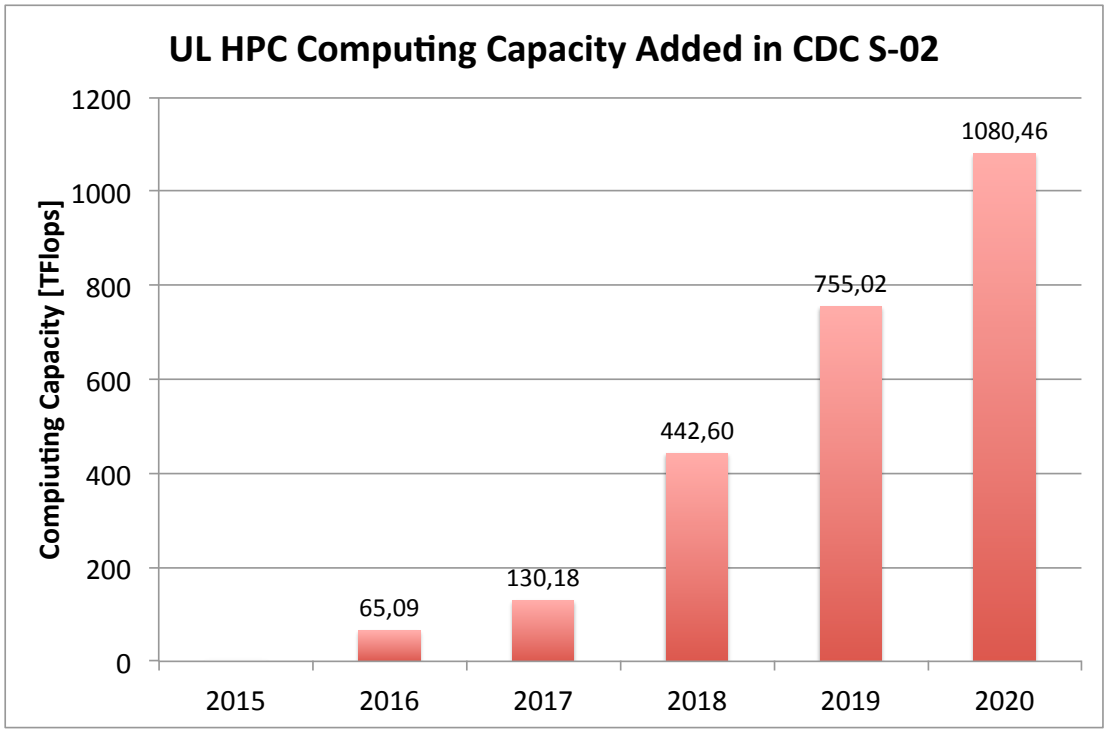
- cf Newsletter: OS/System upgrade
- Storage / Portal consolidation
  - ↪ No way to further extend the HW equipment
  - ↪ QoS, Establish UL as national HPC Center of Excellence

Coming Soon (~~2015~~ 2016)

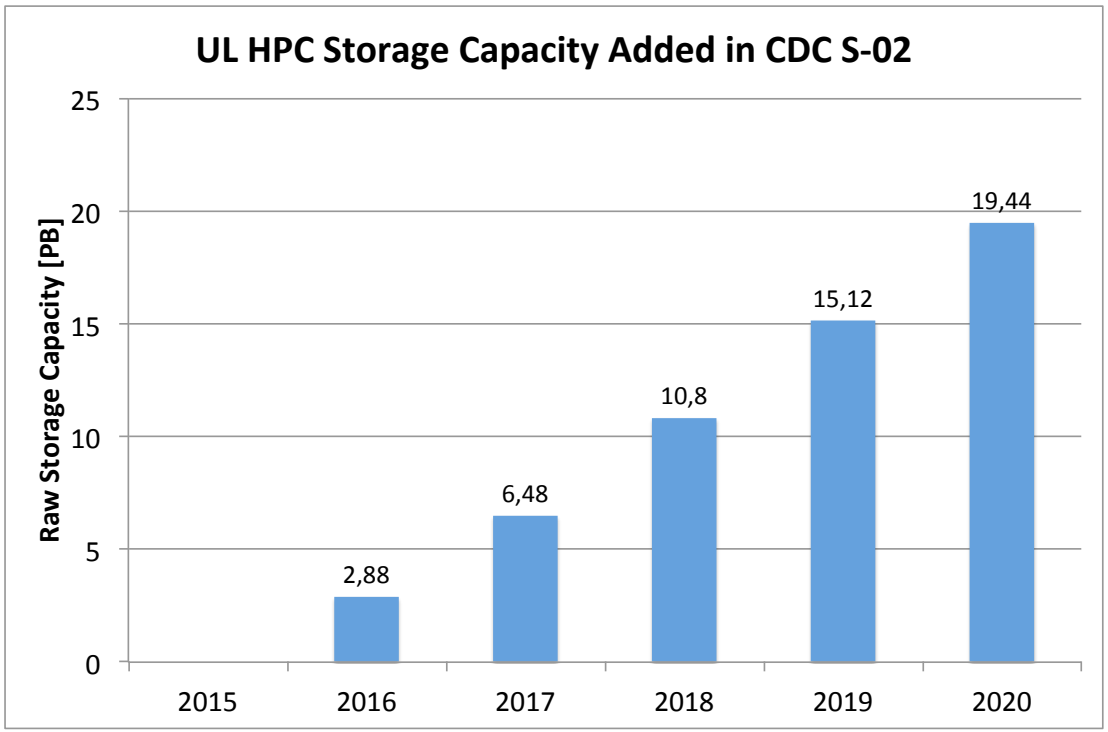
- Belval *Centre De Calcul* (CDC)
  - ↪ 5 new server rooms (3 storage, 2 HPC)
  - ↪ Pending discussions with Fond Belval to re-justify everything

- **Obj.**: Prepare 2 rooms (1 HPC, 1 Storage) by 2020
  - ↪ Budget: $\simeq$ 4M€ per year

UL HPC Planning 2015-2020



UL HPC Planning 2015-2020



UL HPC Planning 2015-2020

- Funding CDC is **mandatory**
  - ↪ Data Center providers (EBRC, LuxConnect etc.) not adapted
    - ✓ **do not have** HPC-ready cabinets (80 kW/rack)
    - ✓ thus proposed renting price is prohibitive
  - ↪ Cloud platforms (Amazon etc.) only able to absorb part of the needs
- **Computational Science** initiative
  - ↪ part of the Digital Strategy for the UL
  - ↪ pending PRIDE call / Doctoral School etc.
- **National HPC initiative**
  - ↪ discussion in progress (MECE, MESR)
  - ↪ **Obj**: national HPC Center of Excellence (CoE)

Cost Model

- UL HPC Platform funding **should** evolve
  - ↪ transition from a free service model to a mixed model
    - ✓ with paying and non-paying tiers
  - ↪ key for providing HPC services at the national level
- You shall also budget your usage upon new project proposal

Cost Model

- UL HPC Platform funding **should** evolve
  - ↪ transition from a free service model to a mixed model
    - ✓ with paying and non-paying tiers
  - ↪ key for providing HPC services at the national level
- You shall also budget your usage upon new project proposal

Cost policy

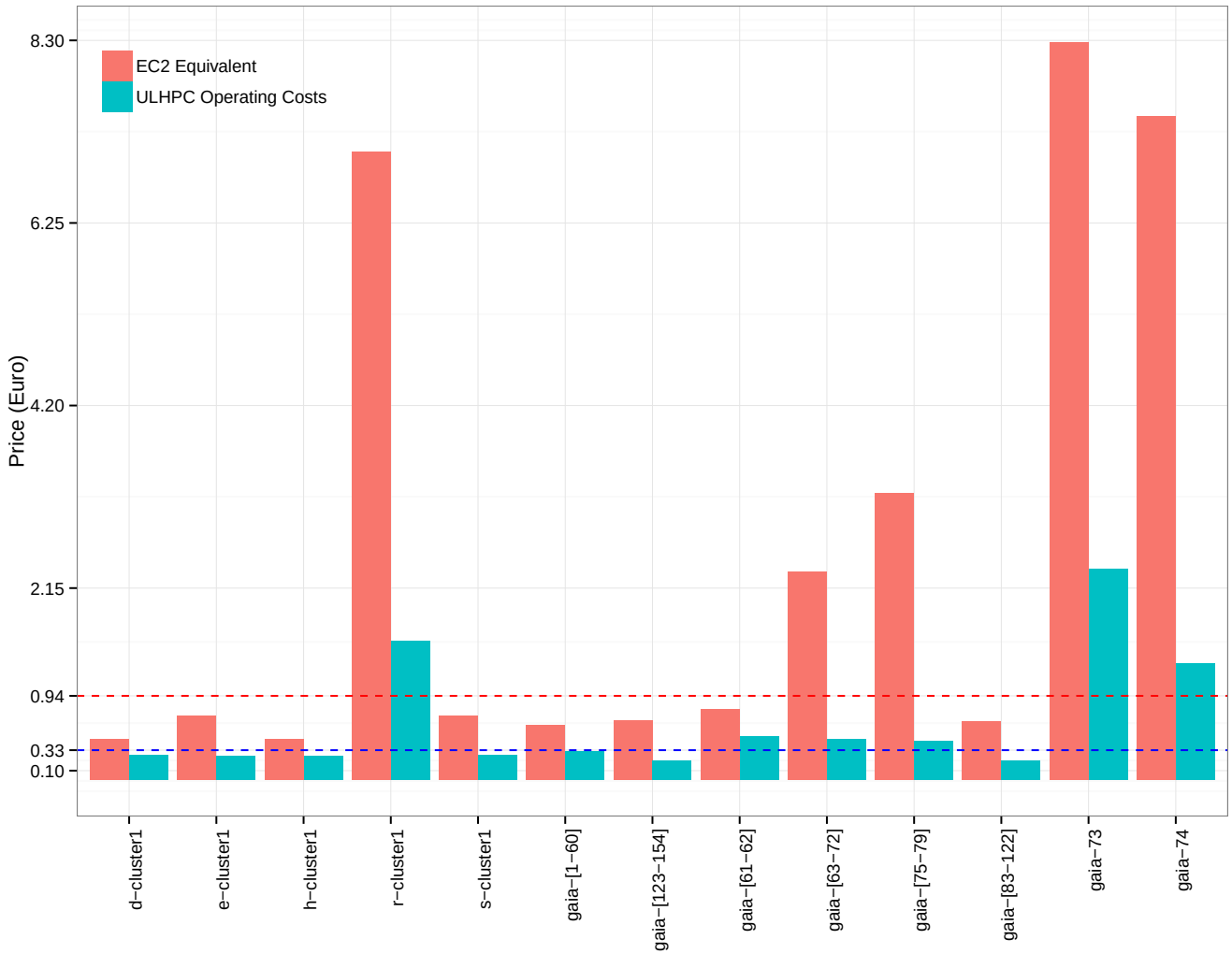
- no charge to the actors of the public research sector
  - ↪ **only** for internal research projects
  - ↪ UL Research Units & ICs, LIST, LISER, LIH
- the same actors **will** be charged for externally founded projects
  - ↪ FNR, European projects, projects with industry

Cost Model

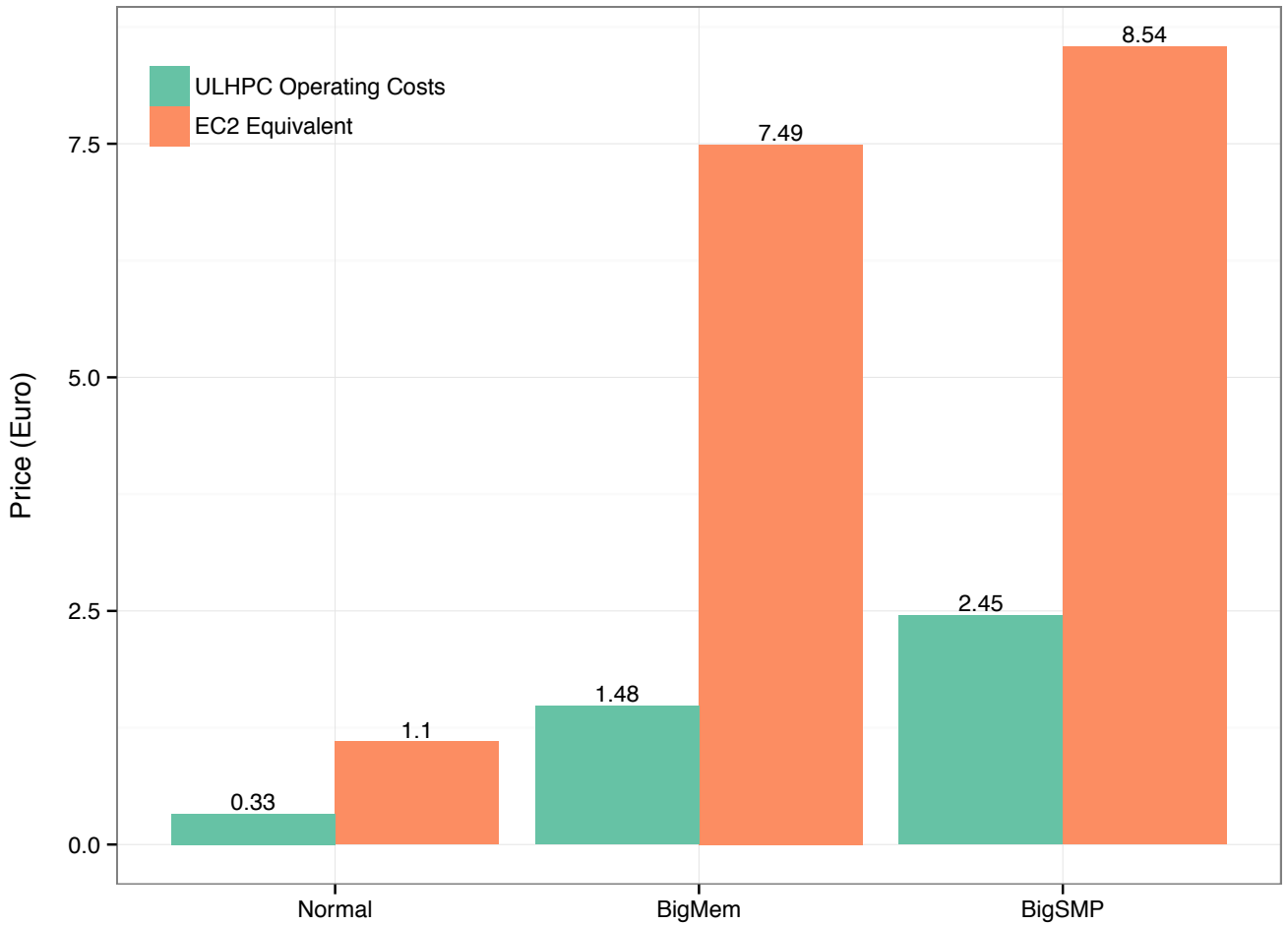
- Pricing units are in the form of usage credits
  - ↪ under a monthly accounting period.
- Two types of credits:
  1. 1 computing credit of class "X" = 1 CPU core for 1 hour
     - ✓ on a resource class "X"
  2. 1 storage credit = 1 TB of storage for 1 month.
     - ✓ 3 storage credits (thus maximum 3TB) for free (each month);
     - ✓ Additional credits: 1000€

Class	Description	Credit Price
normal	Regular HPC resource	0,33 €
bigmem	Regular HPC resource with huge RAM ($\geq$ 1024 GB)	1,48 €
bigsmp	SMP node ($\geq$ 16 sockets) with a huge RAM ($\geq$ 1024 GB)	2,45 €

Computing Credits Prices



Computing Credits Prices



Questions?

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